A Complete Bibliography of Publications in the *Journal of Mathematical Chemistry*

Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA

Tel: +1 801 581 5254

E-mail: beebe@math.utah.edu, beebe@acm.org,
beebe@computer.org (Internet)
WWW URL: https://www.math.utah.edu/~beebe/

24 October 2025
Version 1.45

Title word cross-reference

$(1, 1, 1)$ [2593]. $(1, 12)$ [614]. $(2 + 1)$ [3020, 3016, 3112]. $(2n + 1)$ [1486]. $(3 + 1)$ [3408]. $(\delta(x_0 - |x|)/\left|x\right|^{(n-2)/2})(\delta(x_0 + |x|)/\left|x\right|^{(n-2)/2})$ [569]. $(k, 6)$ [849]. $(M_1 - M_2)$ [277]. $(n + 1) \times (n + 1)$ [788]. $(n, n + 1)$ [1176, 1223, 1227]. (p, q) [2199, 2313, 2065]. $(\mathrm{SU2} \times S_n \otimes (\mathrm{SU2} \times S_n)^+)$ [459]. $(p, \vec{q})$ [2177]. $+$ [2743]. $-Ze^2/r$ [1665]. 1 [3106, 942, 1043, 2061, 1000]. 1/2 [400, 501, 502, 523]. 12 [879]. 2 [2940, 3184, 3009, 942, 2923, 2216, 1092, 1067, 2480, 2339, 1118, 1372, 2127, 1592, 1430, 672, 2857, 1864, 2273]. 26 [1182]. $2p$ [2660]. $2s$ [2660]. $2 \times m \times n$ [419]. 3 [942, 1163, 2555, 1791, 1444, 1286, 3036, 586, 1182, 1075, 1380, 2127, 183, 1592, 249, 2791, 1339]. $3, 16$ [191]. $3, 17$ [191]. 4 [2928, 1163, 2491, 2183, 2569, 1298, 194]. 4(3) [3026]. $4f$ [3418]. $4f^{12}$ [2229]. $4f^2$ [2229]. 5 [2981, 1141]. 5(3) [2334]. 5(4) [2143]. $5g$ [3709]. 6 [879, 860, 798]. 60 [322]. $6 \leq n \leq 20$ [322]. 7 [1627]. 72 [1975]. 8 [2569, 806, 2213, 2930]. $[A]_{12}$ [697]. $[A]_n$ [1290]. $[A]_n(S_n)$ [277]. $[n - 1, 1] \otimes [\lambda]L_{nn}$ [322]. $^+$ [3663, 2743]. $^+_2$ [1232]. $^-$ [953]. $^{-11}$ [614]. ^{1} [3583]. ^{13} [134, 192]. ^{15} [2272]. $^1\Sigma_g^+$ [2968]. ^{2} [2968]. $^{2+}$ [1513]. $^{2-}$ [3146]. $^2\Pi$ [953, 1296, 1260]. ^{3} [953, 1296, 1260, 2575].

$^3\Sigma^-$ [2968]. $^3\Sigma_g$ [953]. $^3\Sigma_g^-$ [1296, 1260]. ^{4} [953, 1296, 1260, 2968]. $^5T_{2g}$ [2992]. * [957]. $_{0.8}$ [2376]. $_{1-x}$ [222, 425]. $_{12}$ [1547]. $_{14}$ [3146]. $_{16}$ [1685]. $_2$ [3709, 1080, 2755, 2376, 2304, 3330, 953, 1296, 1260, 1181, 632, 2575, 3640, 498, 1476, 2087, 1069, 2948, 3663, 250, 2641, 3153]. $_{20n}$ [365]. $^+_2$ [3308, 1116, 390, 2743]. $_3$ [3641, 3655, 3417, 498]. ${}_3\vec{F}_2$ [2652]. $_4$ [1393, 2435, 3641, 3640, 2948, 2093, 1435, 1209]. $_{47-x}$ [1544]. $^+_4$ [2093]. $_5$ [2753]. $_6$ [3146]. $_{60}$ [2755, 1565, 1442, 1732]. $_8$ [1435, 1209]. $_h$ [631]. $_N$ [2030, 1442]. $_x$ [1080, 222, 425, 1544]. $_y$ [498]. A [1084]. $A + A \leftrightarrow C$ [2913]. $A + B \to C$ [2019]. A_2 [1067]. A_6 [1327]. A_α [980]. $A \circ A^{-T}$ [3043]. α [1492, 3384, 438, 1350, 1456, 1599, 1600, 183, 1913]. $\alpha + \beta$ [1913]. $\alpha - t$ [447]. α/β [1913]. $A \to B$ [1306]. B [1459, 1460, 651, 758]. $B_{m'}m^j(\beta)$ [1511]. B_n [980]. $\mathrm{B} \cdots \mathrm{A} \cdots \mathrm{C}$ [1330]. β [414, 855, 183, 1913]. c [2081]. C_6 [3051]. $\mathcal{P}$ [2505]. $\cdots$ [1018]. $\chi(r, r')$ [3643]. D [2465, 587, 1812, 2915, 2916, 3444, 2668, 2726, 1436]. $D(^j)$ [204]. D_{6h} [1251]. D_n [3339]. e [3474, 1163, 1493, 2560, 2827]. ℓ [2671]. $\ell \neq 0$ [1280]. $\exp[-\alpha(t-\tau)]\mathrm{daw}\{[\beta(t\tau)]^{1/2}\}$ [1955]. $\exp[-\alpha(t-\tau)]\mathrm{erex}\{[\beta(t-\tau)]^{1/2}\}$ [1955]. F [940, 179]. $f(E)$ [3059]. $\frac{1}{r_{ij}}$ [1414, 1407]. G [2068, 2373, 441, 442, 443, 2047, 3210, 2023, 1939, 1938, 1327]. $G(3,1)$ [602]. G^q_{-ns} [1379, 1471]. γ [183, 3314]. H [3254, 3133, 1615]. $h \leq 13$ [274]. $H\overline{D}$ [758]. $I(t)$ [996]. $I(t^\beta)$ [996]. I_h [592]. I_i [277]. J [3205, 3206]. j_3 [2873]. K [2611, 685, 295, 3223, 1506, 2374, 1310, 1012, 1221, 3254, 1317, 3133, 1109, 1148, 711, 892, 1120, 1345]. $K(m,n,p)$ [3321]. $k > n/2$ [696]. k^* [843]. K_3 [40]. K_a [1634]. K_{ow} [2864]. l [1556]. $L_2(9)$ [1327]. L_p [2286]. L_q [2350]. (α, c) [2478]. $\left\{\left[\tilde{\lambda}\right] : p \leq 2^2\right\}(\mathrm{SU2} \times S_n)$ [459]. $\left\{\sum_v T^k(v) \to \sum_{\tilde{\lambda}'} \Lambda_{\cdot,\tilde{\lambda}'}[\tilde{\lambda}']\right\}$ [696]. $\left\{\tilde{\mathbf{H}}_v\right\}$ [459]. $l \times m \times n$ [508]. M [3639, 3023, 1498]. $\mathbf{R}^3 \times \mathcal{M}$ [2007]. $\mathbf{R}^4$ [1819]. $\mathbf{R}^n$ [634]. $\mathbf{CD4}^+\mathbf{T}$ [2626]. $\mathbf{P2/m}$ [2586]. $\mathcal{PT}$ [3496]. $\{\mathcal{S}_{\infty\in} \supset \cdots \supset [\in]\mathcal{S}_\in\}$ [697]. $\mathcal{S}_\backslash$ [1290]. O(3) [3296]. $\mathrm{Q_c}$ [2342]. $\mathrm{Q_p}$ [2342]. $\mathrm{Q_x}$ [2342]. SO(3) [3296]. $\mathcal{P}$ [2628]. N [2940, 681, 914, 984, 2634, 3255, 2468, 1914, 276, 95, 194, 2336, 1645, 1027, 1407, 519, 749, 1688, 3481, 2330, 2485, 1892, 1202, 1893, 3071, 920, 919, 971, 1017, 1167, 1471, 1603, 1737, 1498, 1574, 2127, 2126, 854, 2613, 1290, 636, 701, 322, 525, 615, 1438]. $n \leq 7$ [277]. $n \times n$ [788]. O [1418]. ω [1492]. $\overline{\mathrm{U}} \times \mathcal{P}$ [696]. P [3378, 3400, 3471, 3364, 3302, 3370, 3426, 1938, 1492, 1753, 277, 356, 545]. ϕ [2560]. π [492, 978, 1268, 3474, 909, 1163, 1493, 2560, 2861, 2827, 1226, 286, 88, 2918, 1262, 2789, 985, 16, 1006, 3719, 2084, 1210, 933]. $p \to \infty$ [2286]. Ψ [3568]. Ψ^α [1014, 1321, 1659, 1475]. PSL(2, 7) [2915, 2916]. Q [1938, 2879, 491, 2445, 3273, 3389, 452, 1614]. Q^q_{ns} [1460, 1471, 1459]. r [2852, 3628]. $R_{n\ell}(r)$ [3545]. ρ^- [1243, 1049]. $\to$ [953, 2743]. S [3709, 2669, 1261, 1232, 3628]. S^2 [547]. S_{2n} [811]. S_4 [40]. S_5 [40]. S_n [3339, 277, 525, 555, 697, 615]. S_z [547]. $\mathrm{SiO_2}$ [2965, 3053]. $\mathrm{SO}(3) \times S_n$ [277]. SU(2) [204]. $\mathrm{SU}(2) \times \mathcal{S}_{\backslash \geq \infty \in}$ [696, 697]. $\mathrm{SU}(2 \geq m \geq 4) \times \mathrm{S}_{10} \downarrow D_5$ [614]. $\mathrm{SU}(m \leq n/2) \times S_n \downarrow \mathcal{GNMR}$ [525]. $\mathrm{SU}_q(2)$ [491]. T

[2905, 183, 805, 1438, 3628]. $T(2,n)\#C(2,r)$ [2882]. $\Theta_{\ell m}(\theta)$ [3648]. $\rightarrow$ [1296, 1260, 2968]. $\mathrm{U}(n_1+n_2) \supset \mathrm{U}(n_1) \times \mathrm{U}(n_2)$ [363]. υ [276]. υ [811]. $V(r) = -V_0(r/a_0)^{2\nu-2}, 0 \leq \nu \leq 1$ [841]. $V(r) = V_0(r/a_0)^{2\nu-2}, \nu \geq 1$ [840]. $\varepsilon = 1$ [2199]. φ [1493]. ϱ [3681]. $\vec{I}_h$ [3145]. W [2644, 2905]. $\widetilde{\mathbf{H}}_v$ [811]. X [1290]. $X + Y \rightarrow P$ [738]. $x_0 + |x|$ [685]. $x_0 - |x|$ [685]. $X_r(q)$ [409]. $y'' = f(x,y)$ [3081]. Z [1665, 237].

-1 [1621]. **-4** [1102]. **-alkanes** [636, 701, 2940]. **-androstanediones** [191]. **-angle** [2611]. **-antimagic** [2726]. **-ary** [3071]. **-aryl-** [194]. **-aryl-2** [194]. **-Auxiliary** [811]. **-Body** [1118]. **-bonding** [492]. **-bonds** [985]. **-Cages** [849]. **-calculus** [3389]. **-car** [614]. **-carbon** [438]. **-catalyzed** [1170]. **-cells** [2626]. **-chaos** [2177, 2199, 2313, 2628, 2065, 2505]. **-circulant** [2852]. **-circumscribed** [2613]. **-Compatible** [811]. **-confused** [1688]. **-conjugated** [3719]. **-connected** [1163]. **-correlation** [1490]. **-counting** [237]. **-Coupled** [3206, 3205]. **-coverable** [295]. **-Cycle** [843]. **-D** [1092, 2339, 1141, 1043, 1864, 2061]. **-deformed** [2879, 2445, 3203, 1614]. **-dependence** [1645]. **-derived** [459, 555]. **-dihalides** [1694]. **-dimensional** [3481, 1893, 3016, 3112, 1892, 914, 984, 2634, 3255, 2468, 2465, 587, 1812, 2336, 2668]. **-Dimensions** [942]. **-edge-cuts** [1627]. **-Electron** [2084, 286, 1262, 2789, 1006, 1210, 95]. **-electrons** [978, 1268, 2918, 933]. **-ETO** [1659]. **-ETOs** [1014]. **-exponential** [1475]. **-factor** [1000]. **-family** [2478]. **-fold** [1290]. **-fractional** [3639]. **-fullerene** [2932]. **-fullerenes** [1919]. **-function** [3709, 2644]. **-furylethylene** [1430]. **-graphene** [3568]. **-graphs** [179, 1176, 1223, 1227, 1222]. **-Hull** [183, 183]. **-hydrocarbon-iron** [88]. **-hydroxyflavone** [249]. **-independent** [1148, 711]. **-invariant** [1290, 697]. **-Invariant-Based** [811]. **-matchings** [1148, 711]. **-means** [2081]. **-membered** [1914]. **-meshes** [1436]. **-methoxyethanol** [3184]. **-methoxyethanol/2-ethoxyethanol** [3184]. **-methyltransferase** [1418]. **-mixing** [1049, 1243]. **-modules** [525]. **-network** [16]. **-norms** [2286]. **-ol** [2940]. **-ones** [1067]. **-packing** [3254, 3133]. **-particle** [1407, 749]. **-particle-hole** [2068, 2373, 2047, 3210, 1939]. **-partition** [3254, 3133]. **-pendant** [1120]. **-phenylene** [1753]. **-Phosphate** [798]. **-Polynomials** [855]. **-polyphenyl-** [1492]. **-pyridones** [194]. **-quinododimethides** [1492]. **-quinolone** [194]. **-radial** [1350, 1456, 1599, 1600]. **-regular** [1182]. **-Rényi** [3273]. **-representability** [681]. **-representable** [276]. **-Resonance** [892, 2374, 1012]. **-resonant** [1221, 1345]. **-rotator** [491]. **-row** [3709]. **-sequences** [1219]. **-sets** [2023]. **-sextet** [2084]. **-skeletons** [3145]. **-Slater** [1471, 854, 1261]. **-Slater-Type** [920, 1027]. **-space** [356, 545]. **-space-time** [3051]. **-spherical** [3628]. **-Stable** [3400, 3378, 3471, 3364, 3302, 3370, 3426, 1084]. **-state** [2671]. **-states** [1556]. **-step** [2213, 2930]. **-symmetries** [1251]. **-th** [3023]. **-times** [1310, 1317]. **-tridiagonal** [3223, 3379]. **-tuples** [277]. **-type** [1232]. **-uniformly** [3681]. **-valent** [586]. **-wave** [2669]. **-weighted** [441, 442, 443].

/non [1019, 1156].

0.5 [3205]. **0.5KB** [3206]. **09** [1688].

1 [3722, 763, 2319, 3627, 1746, 440]. **1-biradicals** [687]. **1-separation** [3301]. **1-Triradicals** [813]. **1.5** [2602]. **1.5T** [3205, 3206, 3570]. **10.1007/s10910** [1483]. **10.1007/s10910-008-9398-z** [1483]. **14T** [3320, 3358]. **14th** [3480]. **17** [2887]. **18** [3027]. **19** [3646, 3631, 3629]. **1D** [3308]. **1H** [194, 1102].

2 [764, 2320, 2030, 1976, 3527, 3194, 594, 1102]. **2-** [1102]. **2-b** [2420]. **2-ethoxyethanol** [3184]. **2-level** [3459, 3559]. **2-phenyl-2H-chromen-4-ol** [1976]. **2-thiazolyl** [1621]. **2014** [2476]. **2017** [2886]. **2018** [3017, 3015]. **2019** [3099, 3102]. **298.15** [2940]. **2D** [3676, 3189, 3552]. **2H** [1976].

3-Point [3406]. **3-step** [3569]. **3D** [1180, 3460, 3469]. **3rd** [908]. **3T** [3292].

4 [3529, 305, 933]. **4-dihydro-4-oxo-1-** [1621]. **4-regular** [3263]. **42** [1455]. **4B** [3132].

5 [1102]. **5-b** [2420]. **5-dihydro-1H-3-oxoimidazol-1-oxyl** [1102]. **5-pyrimidinyl** [1102]. **5-tetramethyl-4** [1102].

6 [978]. **6D** [3085]. **6D-hypercube** [3085].

8-naphthyridines [1621]. **8th** [384].

= [3641, 1096].

ab-initio [1546]. **AB-type** [3583]. **ABC** [2753, 2948, 501, 502, 2736, 2821]. **ABCD** [501, 502]. **ability** [6]. **absolute** [1713, 1792, 2358, 2452, 3128, 3064]. **absorbed** [2492, 3136]. **absorbs** [2327]. **absorption** [2842, 3020]. **abstractly** [2542, 2784]. **accelerated** [1841, 2073, 2115]. **accelerating** [3539]. **acceleration** [1872]. **accelerators** [2489]. **acceptable** [1312]. **acceptance** [530]. **accomplished** [3073]. **according** [1858, 213, 212, 279, 1360]. **accounting** [2155, 3070]. **accumulation** [2019]. **Accuracy** [2339, 338, 2169, 1634, 3559, 3198]. **Accurate** [2282, 2688, 1321, 2738, 3488, 1344, 3664, 521, 3155, 3477, 3702, 1764, 2457, 3508, 958, 554, 1947]. **acetic** [2631, 1844]. **achieved** [1454, 500]. **achiral** [110, 439, 464, 490, 327]. **achirality** [454]. **acid** [1700, 1951, 2631, 1844, 1656, 2685]. **acidic** [2225, 450, 3434]. **acids** [3007, 991, 3524, 1733]. **acrylic** [1530]. **actinide** [3204]. **Action** [834, 1800, 2249, 3000, 1878, 3296, 453, 510, 1853, 2308, 2635, 3309, 2250, 1215, 1985, 1588, 1301]. **actions** [3740, 3742, 759]. **activated** [2786]. **activation** [1932, 1729, 2376, 1191, 1723, 1724, 3669, 1691, 1925, 3059].

activator [3103, 3589, 3055]. **activator-inhibitor** [3103, 3055]. **active** [169]. **activities** [1704, 2133]. **Activity** [1067, 1763, 319, 186, 2831, 128, 165, 1200, 3460, 1801, 92, 3623, 2265, 2442, 2601, 1621, 2133]. **Acyclic** [1031, 1090, 853, 868, 171, 260, 86, 643, 1298, 1239, 626, 1601]. **Adams** [3567, 3714, 3739]. **Adapted** [2937, 2373, 1393, 2435, 2710, 2847, 2047, 412, 2260, 3210]. **Adaptive** [3564, 1955, 2290, 3516, 1491]. **Adding** [2900]. **Addition** [1014, 1028, 1039, 1050, 1205, 1284, 1447, 1595, 1659, 1769, 1907, 3348]. **Additive** [2714, 1624, 1565, 1622, 3405, 440]. **additivity** [329, 331, 409]. **addressing** [3608]. **ADI** [3603]. **adiabatic** [1945, 2985, 802]. **adjacency** [462, 3003]. **adjacent** [118, 587]. **Adjoint** [393]. **adjoints** [969]. **adjustable** [1983, 465]. **adjustments** [1943]. **Adomian** [2492, 2284]. **adopting** [1465, 1466]. **adsorption** [2553, 3463, 3722, 1897, 2976, 1935, 2085, 1001, 1194, 1303, 1404, 3144]. **advanced** [1540, 3310]. **Advances** [1923]. **Advancing** [3654]. **Advection** [663, 2488, 3279]. **advection-diffusion** [2488]. **Advection-dispersion** [663]. **aerogel** [2830]. **aerosols** [2656]. **affinity** [1746, 2300]. **after** [2071]. **again** [399, 3380]. **against** [515, 1801, 3001, 3098]. **AGDC** [1762, 2494]. **age** [1583]. **agent** [2980]. **agents** [1538, 3527]. **aggregate** [950]. **Aggregates** [943, 1268, 619, 1685]. **aggregation** [3628]. **aging** [2430]. **aided** [171]. **air** [1856, 1935]. **air-water** [1856, 1935]. **Airy** [639, 871]. **Al** [222, 425, 173]. **alcohol** [1534]. **Alcohols** [1170, 266]. **Aldehydes** [1106]. **Alder** [2094]. **aldose** [193, 1323]. **Algebra** [778, 1060, 2885, 2986, 421, 422, 423, 424, 441, 442, 443, 139, 140, 2089, 158, 2132, 353, 354, 717, 2230, 277, 3162, 3169]. **Algebra-based** [3169]. **Algebraic** [755, 915, 817, 896, 1128, 445, 225, 3174, 659, 806, 3740, 548, 800, 933, 906, 1745, 2524, 2549, 2673, 2662, 2691, 557, 2777, 675, 283, 2598, 53, 3078, 2365, 2552, 3382, 473, 3524, 2507, 2511, 967, 1099, 713, 636, 701, 2574, 210, 956, 517, 2648, 732, 2719, 727]. **algebraic-combinatoric** [636, 701]. **Algebras** [811, 217, 97, 332, 363, 3191, 1290]. **Algorithm** [842, 2939, 3084, 2863, 921, 1062, 1674, 1933, 1927, 3284, 2226, 3224, 2823, 3713, 2777, 2290, 462, 2435, 3006, 2597, 271, 3530, 3324, 2494, 3701, 2063, 1707, 296, 1196, 953, 2026, 2139, 2401, 3149, 3223, 3381, 3464, 3593, 1921, 1497, 3440, 3113, 2531, 3397, 446, 1426, 3131, 195, 3061, 2583, 2851, 3037, 3217, 3152, 1841, 2234, 1331, 1043, 3063, 1677, 1684, 2081, 2975, 2627, 2799, 3102, 2971, 3187, 2994, 1644, 3134]. **Algorithmic** [794, 429, 3535, 388, 717]. **Algorithms** [895, 2804, 740, 3696, 3043, 394, 455, 2807, 3165, 3702, 532, 2351, 324]. **Aliasing** [2216]. **alignment** [3617, 1267, 2200, 2142]. **alignments** [438]. **aliphatic** [3625]. **alkali** [2931]. **alkane** [3644]. **alkanes** [2940, 260, 216, 445, 1229, 1579, 3462, 94, 47, 164, 636, 701, 517]. **alkenes** [603]. **Alkyl** [813, 603, 687, 3462]. **Alkylcyclobutadienes** [813]. **alkylcyclopropanes** [687]. **alkynes** [603]. **all-** [1913]. **all-benzenoid** [181]. **allelopathy** [1725]. **Allen** [3517]. **allene** [1694]. **allene-1** [1694]. **allenes** [2371, 2372]. **allosteric** [1786]. **allotrope** [589, 2915, 2916]. **Allotropes**

[1010, 2387, 668]. **allyl** [2041]. **almost** [2386, 3393, 1895, 3595, 2822, 2280]. **almost-equienergetic** [2280]. **along** [3626, 1969]. **Alpha** [330, 3132, 3503, 3576, 3542, 1764, 692, 2604]. **alpha-hulls** [692]. **alpha-oscillators** [2604]. **alphabet** [1580]. **already** [359]. **altans** [2622]. **ALTEC** [2573]. **altering** [2473]. **alternant** [329, 1753, 1262, 206, 325]. **alternants** [330]. **Alternate** [1772, 1770]. **Alternating** [1016, 3075, 2933, 1327]. **Alternative** [1073, 678, 3344, 3135, 2415, 2238, 3545, 698, 519, 3098, 1193]. **Alternatives** [1282]. **altitude** [2873]. **altitude-** [2873]. **Aluminium** [1152, 3307]. **ambient** [955]. **americium** [1925]. **Ames** [2902]. **amino** [1733]. **ammonia** [2220, 2321]. **Among** [924, 819, 932, 2918, 992, 1469]. **amongst** [956]. **Amount** [890]. **Amperometric** [828, 880, 934, 901, 1849, 3011, 1386, 1606]. **amphicheiral** [370]. **Amplitude** [3589, 1740, 1538, 2530, 2769, 2926]. **amplitude-phase** [2530, 2926]. **analog** [3051, 394]. **analogs** [424]. **analogue** [3382]. **analogues** [3710, 1441]. **Analogy** [873]. **analyse** [539]. **analyses** [3124, 747]. **Analysis** [2463, 828, 934, 2154, 866, 930, 858, 1034, 848, 200, 3309, 3519, 3725, 2786, 2652, 809, 2415, 477, 719, 2285, 3354, 1024, 1504, 1356, 1310, 3595, 3667, 1248, 2693, 830, 773, 1254, 1317, 2774, 798, 997, 2632, 2804, 3023, 2895, 36, 3401, 2311, 1849, 2485, 3428, 2071, 1807, 3602, 722, 3247, 3287, 2314, 1202, 1256, 1362, 1277, 2800, 3660, 411, 2464, 3410, 3583, 2761, 3258, 529, 2555, 2465, 2337, 2841, 3157, 2168, 12, 1856, 1225, 3514, 3448, 1191, 2017, 1707, 1241, 2186, 3445, 2146, 3626, 1334, 1377, 1562, 1660, 3036, 1057, 1846, 3712, 1741, 3035, 1842, 1515, 56, 1586]. **analysis** [1965, 2767, 84, 3436, 2681, 1194, 1303, 2480, 357, 1219, 2339, 2219, 2631, 2716, 333, 449, 2763, 3478, 3151, 1723, 2679, 1584, 2946, 3728, 156, 183, 257, 315, 307, 2752, 1204, 2776, 104, 2079, 249, 1675, 2234, 2013, 3719, 1501, 551, 583, 1647, 950, 3533, 2246, 2333, 592, 1512, 1691, 247, 1872, 3509, 3672, 3189, 11, 20, 2315, 3359, 3665, 1583, 738, 2098, 2033, 2921, 3693, 2607, 537, 1573, 2265, 2442, 2601, 1621, 2436, 48, 116, 1193, 1285, 3554, 3121, 484, 64, 65, 1789, 3470, 3670, 1314, 1273, 1520, 1563, 2051, 2354, 1656, 3317, 1558]. **Analytic** [470, 145, 645, 379, 2064, 2801, 3221, 2867, 600, 2416, 356, 3664, 1863]. **Analytical** [3245, 2034, 3385, 990, 366, 3207, 2802, 2999, 3466, 917, 938, 1017, 1091, 1483, 1334, 1995, 3011, 2541, 2725, 2390, 1861, 2261, 2717, 1482, 1511, 3290, 2119, 1641, 1261, 3423, 2613, 3412, 3707, 881, 1839, 1862, 1438, 3639, 2658, 2032, 2330, 2887, 3086, 2343, 1315, 501, 502, 523, 2873, 3486, 135, 1957, 980, 999, 3678, 1874, 1190, 1710, 608, 2014, 2499, 3308, 2583, 1693, 2349, 2073, 2221, 2207, 686, 601, 2338, 1434, 2092, 2413, 2978, 3272, 2135]. **Analytical-numerical** [2119]. **analyzed** [2998]. **Analyzing** [1082, 3216, 3634, 1651]. **ancient** [3324]. **and/or** [2938, 2908, 2943, 2851, 2855, 2250, 2954]. **Anderson** [1803]. **androstanediones** [191]. **angle** [1556, 1494, 408, 2035, 2611, 1670]. **angle-dependent** [1556, 1494, 2035]. **angles** [1376, 461, 2366]. **Angular** [1171, 1060, 2034, 617, 1814, 944, 2132, 1884, 1350, 1456, 3290, 1837, 2769].

Anharmonic
[2817, 797, 475, 718, 1094, 2642, 3010, 3313, 2349, 2275, 2552, 2554, 3295, 3045]. **anharmonicities** [725]. **anhydrase** [1200]. **Animals** [1025, 292, 238, 399, 177, 257, 123]. **Anions** [861]. **Anisotropic** [3251, 481, 2724, 2079]. **anisotropy** [3303, 3451]. **ANN** [3284]. **ANN-MATOPT** [3284]. **annealing** [2290, 2439, 561]. **ANNs** [3074]. **annulene** [2587]. **annulene-** [2587]. **annulenes** [40]. **annuli** [2609]. **anomalous** [2376, 3103, 3055, 2405]. **Ansatz** [2033, 2338, 3382, 1407, 1414]. **ant** [3530]. **antagonistic** [3340]. **Anti** [1178, 3229, 1429, 3460, 3527, 1263, 2958]. **Anti-forcing** [1178, 1263, 2958]. **anti-gastric** [3460]. **anti-Kekulé** [3229, 1429, 1263]. **anti-neoplastic** [3527]. **antibiotic** [1301]. **antibody** [2300]. **antibody/antigen** [2300]. **anticancer** [1621]. **Anticipated** [3212]. **antidiagonal** [3291]. **antigen** [2300]. **antimagic** [2726]. **antiprisms** [3710]. **Antisymmetric** [973]. **antisymmetrized** [3520]. **antiviral** [3631]. **any** [2034, 1582, 3706, 1171, 2721, 670, 1542]. **anything** [1926]. **Apparent** [1320, 690, 2473]. **appearing** [3697]. **Applicability** [3486, 1135, 3019]. **Application** [2237, 996, 2986, 2516, 1034, 319, 1255, 3427, 1366, 1595, 937, 1134, 724, 1067, 1200, 3499, 747, 923, 1045, 1118, 1705, 1820, 661, 125, 156, 1430, 513, 514, 593, 166, 1386, 870, 1774, 893, 2300, 773, 906, 522, 622, 732, 389, 390, 2595, 1674, 2647, 259, 2672, 990, 367, 2290, 491, 2386, 1395, 2435, 2304, 2337, 2020, 675, 1530, 628, 1444, 2996, 3708, 110, 1753, 1887, 1888, 3627, 2961, 1481, 93, 266, 2767, 2972, 1001, 134, 1749, 1702, 1426, 3692, 566, 2864, 2717, 3403, 44, 307, 1667, 1006, 214, 3434, 1980, 1036, 2234, 2013, 1365, 2429, 1844]. **application** [1355, 1993, 1899, 1862, 2023, 2805, 350, 1273, 1563, 1558, 2368, 1925]. **Applications** [3339, 857, 9, 394, 344, 3521, 795, 2057, 1060, 2530, 3630, 3683, 1683, 2759, 2895, 3031, 3114, 331, 2663, 639, 1279, 61, 2696, 2928, 2981, 3085, 428, 1453, 1668, 2967, 3602, 105, 595, 3449, 1288, 2103, 456, 1393, 3111, 3258, 2555, 3641, 24, 476, 3352, 3475, 3578, 3666, 2482, 2182, 4, 5, 22, 284, 342, 3725, 1180, 2129, 2763, 2894, 1518, 2903, 1380, 1372, 3522, 3461, 2707, 3267, 1964, 1535, 3045, 3139, 2704, 1407, 1414, 1500, 1845, 245, 584, 3283, 3716, 2966, 116, 1930, 2156, 1364, 3038, 3407, 2235]. **Applied** [1126, 1047, 3742, 2328, 1970, 1258, 2074, 691, 2005, 2751, 2494, 2872, 1603, 2146, 2245, 1842, 2324, 26, 641, 3139, 759]. **Applying** [2357, 3083, 1639, 3074]. **Approach** [886, 898, 931, 838, 820, 796, 1465, 1466, 902, 762, 1680, 429, 1972, 2010, 2397, 2406, 2015, 255, 1777, 1607, 1280, 261, 374, 193, 1770, 423, 2812, 2294, 2468, 3641, 2337, 2160, 2161, 2162, 187, 3504, 1255, 3126, 3313, 3387, 6, 3490, 3437, 3525, 3729, 991, 1229, 2048, 2049, 2298, 2299, 2371, 2372, 2358, 2491, 2477, 2902, 1681, 1886, 2427, 2216, 2319, 2320, 674, 3215, 3282, 1316, 1190, 1710, 3079, 648, 3662, 3334, 3699, 3596, 1741, 535, 3567, 3494, 3379, 388, 1920, 2657, 2686, 2985, 2346, 1750, 2077, 162, 53, 54, 2849, 3319, 3499]. **approach** [2247, 2014, 3078, 1503, 3640, 3471, 3692, 2128, 2129, 2342, 2545, 2716, 3586, 243, 2140, 705, 692, 2365, 2552, 2221, 2115, 2711, 548, 3524, 378, 2332, 1349,

2382, 3295, 960, 642, 70, 2877, 3192, 2532, 3458, 494, 524, 1540, 3412, 1267, 2246, 2405, 3545, 2157, 2638, 2637, 2997, 3281, 3376, 616, 497, 2475, 3612, 3426, 3704, 3177, 324, 1539, 2626, 3059, 522, 482, 3724, 2988, 2277, 1322, 369, 1759]. **approaches** [3646, 1536, 3486, 2710, 2238, 2708, 3190, 3290, 2929]. **Approaching** [2669]. **appropriate** [2417, 3620, 3581, 3591, 3534]. **approximants** [2090, 2160, 2714, 1638]. **Approximate** [1628, 2032, 3699, 1171, 2349, 945, 3332, 1332, 1323, 2335, 35, 1694, 2118, 2253, 1527, 1315, 743, 2360, 2511, 2098, 2267, 2135, 2774, 2719]. **approximated** [2827]. **approximately** [1496]. **Approximating** [769, 511, 648, 3322]. **Approximation** [3105, 2861, 3017, 2849, 3262, 1521, 1542, 2772, 1926, 3713, 3565, 142, 1297, 521, 598, 1973, 2153, 1582, 2181, 3048, 655, 2710, 1765, 3418, 2324, 2811, 3633, 2890, 2733, 243, 3547, 2449, 1918, 3508, 3559, 3444, 2145, 3430, 3488, 189, 3045, 556, 51, 2416, 3405, 2204, 2720, 2854, 3042, 2775]. **Approximations** [793, 782, 3285, 1413, 3722, 3474, 374, 1451, 1770, 1950, 2600, 1855, 1307, 1863]. **APSG** [1829]. **aquaglyceroporin** [2240]. **aquaporin** [2240]. **aquaporin-1** [2240]. **aquaporins** [2220]. **aqueous** [1361, 3524]. **Ar-like** [1773]. **aragonite** [1513]. **Arbitrarily** [767]. **Arbitrariness** [857, 2319]. **Arbitrary** [778, 827, 1153, 837, 2124, 2760, 1366, 1814, 1986, 1660, 515, 228, 2703]. **Arbitrary-rank** [1153]. **Archimedean** [1755, 1709, 1042, 1376]. **architecture** [1524, 1883, 1712]. **area** [385]. **areas** [150, 2883]. **Arenes** [30]. **arises** [3660, 3726, 3705]. **Arising** [842, 1017, 1011, 1084, 2875, 3312, 1471, 2245, 2359, 2882, 2955, 1045, 2974, 2244, 2583, 1861, 3513, 1985, 2507, 2980, 3244, 1519, 2638, 2637, 3327, 3376, 3297, 2626, 2471]. **arithmetic** [3390, 3636, 1609, 3544, 3260, 2756, 2890, 3027, 1630]. **arithmetic-geometric** [3260]. **arithmetical** [1571]. **armchair** [3647, 3734, 1431, 2846]. **Aromatic** [1169, 2237, 3557, 1361, 32, 2084, 3625, 998]. **Aromaticity** [1492, 1422, 978, 3734, 1226, 84, 1610, 1688]. **arrangement** [1336]. **arrangements** [2059, 3357]. **array** [3043, 3422]. **arrays** [2089, 2423, 2707, 1652, 1672]. **Arrhenius** [1451, 3122, 3696, 3669, 1867]. **Art** [1992]. **artefact** [2461, 2462]. **arterial** [2621]. **Artificial** [934, 2264, 193, 456, 2193, 128, 2656]. **ary** [3071]. **aryl** [194]. **ASA** [1973]. **ascent** [2434]. **Asked** [801, 1948]. **aspect** [2452]. **Aspects** [2341, 330, 586, 1713, 1443, 1900, 1287, 1288, 1289, 1805, 2103, 2358, 1699, 157, 589, 2913, 1778, 2509, 184, 3663, 710, 1397]. **assembling** [669]. **assembly** [2862]. **Assessment** [1869, 789, 1699, 3640]. **assist** [81]. **assisted** [25, 2391, 986, 2252, 3675]. **Associated** [3648, 3168, 1757, 2435, 262, 341, 2031, 1500, 1845, 2428]. **association** [1731]. **associative** [2913]. **associative-dissociative** [2913]. **assuming** [983]. **assumption** [3216]. **Astereogenicity** [850]. **Asymmetric** [906, 1713, 2043, 2297, 1319, 1041, 3333]. **asymmetrical** [1932, 1261]. **asymmetry** [369]. **asymptotes** [3303]. **Asymptotic** [3637, 475, 330, 329, 331, 466, 884, 883, 3287, 609, 667, 2973, 805, 1725, 1062, 996, 3232, 2266, 2417, 2282, 2165, 948, 2281, 1570, 3198, 419, 508, 1043, 1638, 2573].

Asymptotically [1005]. **Asymptotics** [2286, 1384, 2170]. **atmospheric** [2873, 2001, 3310]. **Atom** [3399, 3225, 3738, 1669, 1668, 2951, 3442, 3441, 479, 2614, 411, 1736, 2555, 2187, 2183, 2042, 1465, 1466, 852, 1966, 1380, 1372, 2509, 3290, 1043, 2218, 732]. **atom-based** [2555, 1380, 1372]. **Atom-bond** [3399]. **atom-diatom** [3290]. **atom-diatomic** [732]. **Atomic** [1496, 598, 2860, 1151, 3319, 2538, 2669, 216, 1288, 1973, 2131, 2564, 2688, 3424, 1475, 1814, 587, 264, 318, 1327, 3499, 2652, 566, 1773, 689, 688, 3080, 958, 1455, 189, 199, 596, 737, 1488, 1569, 1903, 2627, 2780, 2810, 3371, 2375, 1788, 2260, 3068, 3177, 1330]. **atomic-chains** [2375]. **Atomic-Molecular** [1151, 1455]. **Atoms** [851, 2096, 2130, 918, 691, 2131, 2649, 3489, 3155, 3437, 3411, 1244, 2059, 167, 547, 2324, 2681, 251, 661, 1476, 1645, 1622, 3617, 1300, 1535, 189, 3452, 1727]. **ATP** [3271]. **ATS** [2791]. **attack** [1976]. **Attainable** [338, 559]. **attempt** [1306]. **attenuation** [2912]. **Attraction** [836, 920, 919, 854, 1027, 3372, 971, 1483, 1599, 1600, 1482, 1261, 3362]. **attractions** [2242]. **attractive** [2474, 1786]. **attractivity** [1703]. **attractors** [986]. **attribute** [3628]. **attributes** [3644]. **Aufbau** [1341, 80]. **Augmentation** [788, 2241]. **Augmented** [3530, 1706, 258, 288]. **Author** [716, 741, 765]. **auto** [415]. **auto-coherent** [415]. **autoacceleration** [2388]. **autocatalysis** [1713, 2124, 2568, 2402, 436]. **Autocatalytic** [2682, 1029, 306, 1661, 628, 550, 3560, 1319, 1723, 1724, 641, 518, 2536, 433, 2988]. **Autocorrelation** [848]. **automata** [534]. **automated** [193]. **Automatic** [3066, 1955, 456, 3350]. **automorphic** [2386]. **automorphism** [297, 178]. **autonomous** [2090, 2319, 2320, 2695, 2888, 537]. **autoregressive** [1384]. **autoregulatory** [3332]. **Auxiliary** [917, 811, 980, 1379, 1471, 1329, 1511, 1459, 1460]. **Average** [3323, 3476, 153, 2449, 3388]. **averages** [2394]. **Averaging** [871, 785, 639, 2701, 2740, 1398]. **avian** [1651]. **avoided** [1945]. **avoiding** [1406, 2289, 2303]. **away** [2690]. **Axes** [749, 2661]. **axial** [87, 355]. **axiomatic** [735]. **axis** [3353, 222]. **axisymmetric** [3470]. **azeotrope** [3427]. **azines** [1251].

B [2304, 3650, 2420, 3607, 3726, 1895, 3125, 3304, 3572, 3197, 614]. **B-boranes** [614]. **B-Spline** [3650, 3726, 3125, 3304, 3572, 3197]. **B-splines** [3607]. **Ba** [1513]. **backbone** [195]. **backbones** [287]. **Background** [916, 435, 1961]. **Backus** [1006]. **backward** [3406, 3212]. **Bagley** [3054]. **Baker** [217]. **Balance** [777, 1533, 3365, 1990, 3138]. **balanced** [2246, 131, 695, 1825]. **Balancing** [870, 3580, 2520]. **Ball** [2904, 2728, 3494]. **ball-milling** [3494]. **Ballena** [3015]. **Banach** [2895, 3453, 3107]. **Band** [825, 2420, 425, 304, 3334, 1253]. **bands** [2239, 1397, 1044, 1054]. **Bare** [401, 1665, 228]. **barometric** [1640]. **barrier** [2032, 2840]. **barriers** [2412]. **Barycentric** [219]. **base** [2859, 2750, 689, 1976, 1434]. **Based** [815, 1079, 939, 1141, 809, 811, 1821, 1062, 3116, 1797, 1696, 1697, 2934, 2945, 3200, 2189, 2647, 2663, 2965, 3686, 1352, 974, 2829, 1546, 208, 260, 3481, 2311,

649, 1813, 2964, 1139, 3201, 2825, 1351, 977, 3259, 2420, 3099, 3100, 3517, 2555, 2597, 3641, 1472, 2411, 1123, 1105, 1229, 1853, 3143, 2477, 202, 2245, 310, 3507, 32, 3446, 3668, 340, 2026, 3149, 3223, 1497, 585, 1699, 165, 3418, 2970, 3084, 3319, 3397, 1778, 1779, 1425, 2863, 1219, 2184, 3377, 1237, 1292, 1336, 2904, 2583, 3008, 3478, 1380, 1372, 1538, 1041, 693, 1717, 1841, 2718, 378]. **based** [2439, 1204, 2776, 3147, 2399, 2102, 1043, 2558, 3533, 1267, 1864, 3209, 3003, 3024, 3194, 2470, 3371, 1863, 1774, 3665, 2200, 3391, 3154, 666, 1947, 3254, 2396, 3169, 3649, 1565, 1551, 1621, 1746, 3622, 1879, 1810, 1539, 1193, 2331, 1376, 1571, 3013, 3121, 3628, 3348, 2883, 1339, 1358, 1558]. **bases** [2435, 3296, 541, 2877, 2241]. **Bashforth** [3714, 3739]. **Basic** [763, 3007, 1379, 20, 3154]. **basics** [2126]. **basins** [3372]. **Basis** [930, 2008, 875, 496, 618, 1655, 193, 1953, 2103, 1393, 3486, 275, 3202, 3606, 2688, 2358, 2451, 3627, 318, 363, 958, 452, 3290, 2057, 3552, 2753, 2948, 1004, 133]. **Batch** [828, 894, 2964, 3436, 3539]. **Bateman** [2379]. **batteries** [1880, 2787]. **Bautin** [3095, 2425]. **Bayesian** [2441, 2158, 2440]. **Bazley** [1282, 1850, 2222]. **BaZrO** [3655]. **BBM** [2582]. **BCIS** [3132]. **BCIS-4B** [3132]. **Bcl** [3527]. **Bcl-2** [3527]. **BCS** [600, 635]. **BDF** [3569]. **BDW** [3132]. **BDW-4B** [3132]. **be** [1615, 267, 2207, 1076]. **bed** [1780, 1999]. **Beddington** [1356, 1374, 1340]. **Behavior** [805, 3637, 707, 2614, 3226, 2892, 3182, 2165, 3711, 1935, 948, 1699, 3041, 2113, 3665, 2224, 1248, 1238, 2265, 2442, 694, 2616, 2929, 1577, 3597]. **behaviors** [1687, 1725, 1195, 1371, 1594, 3656]. **Behaviour** [1159, 2478, 2437, 1457, 1458, 198, 2114, 235, 3090, 1913, 983]. **behaviours** [2296]. **bell** [3492, 2952]. **bell-shaped** [3492]. **Belonging** [792, 1913]. **Belousov** [2658, 3226, 2937, 858, 377, 151, 410]. **Belusov** [2313, 1690, 1679, 2228, 2177, 2199, 2559, 2628, 2615, 3140, 2505, 1997, 2065]. **benchmark** [2081]. **benchmarks** [2339]. **Bending** [831, 249, 359]. **benign** [3320, 3358, 3431]. **Benjamin** [3673]. **Benzene** [816, 1169, 523, 1890, 406, 1822]. **benzenes** [2907]. **Benzenoid** [792, 1125, 786, 328, 1140, 398, 1608, 226, 294, 137, 181, 1218, 80, 50, 2664, 2625, 296, 375, 431, 32, 185, 2613, 3213, 616, 75, 2956, 2966, 956, 998, 111, 211]. **Benzenoids** [1178, 869, 978, 41, 1199, 3148, 1375, 2063, 2217, 2325, 1390, 1965, 1964, 2084, 1263, 933]. **benzo** [2420]. **benzvalenes** [2907]. **Berlin** [759]. **Bernstein** [2718, 3297, 3239]. **Berry** [2906, 2028]. **beryllium** [1925]. **Bessel** [3486, 2519, 946, 3156, 713, 3211]. **best** [2991, 3046, 317, 2994]. **Bethe** [27, 3382]. **Between** [886, 752, 831, 879, 844, 860, 922, 1160, 770, 761, 1208, 2220, 1490, 1757, 1268, 3577, 996, 3183, 3104, 1289, 2131, 3004, 424, 2420, 3536, 3260, 1316, 1190, 2308, 2576, 603, 1648, 2169, 1308, 1325, 1884, 2117, 692, 1441, 317, 1349, 1629, 104, 1719, 2147, 1409, 1364, 2366, 1058, 1000, 1967]. **Beyond** [3720, 2181, 3263, 3326, 2792]. **bi** [3588]. **bias** [1364]. **bibliometric** [2766]. **bicriticality** [2932]. **bicubic** [3105, 3017]. **bicyclic** [3238, 976]. **bielectronic** [651]. **bienzyme** [3196]. **Bifurcation** [2841, 1498, 2219, 802, 1373, 761, 1573, 3410, 3157, 3455, 231, 2517, 2242, 2676, 1974, 3518, 537, 433, 1625, 430, 484, 2425, 3635]. **bifurcations**

[3455, 3095]. **bilayer** [3671]. **Bilayered** [1275]. **bilinear** [1372]. **Bimolecular** [814, 1957, 1851, 2561]. **Binary** [2913, 2838, 2940, 1888, 3617, 970, 2461, 2462, 2706, 1557]. **Binding** [222, 1546, 2311, 425, 202, 2127, 2126, 2306, 2621, 1746]. **bindings** [983]. **binomial** [1045, 1764, 2261, 2630]. **binuclear** [1229]. **Bio** [1127, 2300, 1412, 2635, 1302, 1625, 1563, 1387]. **bio-catalytic** [2635]. **bio-chemical** [1625]. **Bio-Layer** [2300]. **bio-polymer** [1412]. **bio-reactor** [1302, 1387]. **bio-sequence** [1563]. **Bio-target** [1127]. **bioactive** [3623]. **Biochemical** [926, 3219, 3220, 1795, 2535, 2659, 1902, 2173, 2223, 2973, 3008, 1985, 1663, 2356, 3656, 1789, 3690]. **biochemistry** [245]. **Biodegradation** [2646]. **Biodiversity** [913]. **bioelectrocatalysis** [1862]. **Bioethanol** [2189]. **biogas** [3668]. **Biological** [874, 1018, 2885, 92, 1273]. **biology** [2696, 246, 3502]. **biomagnetic** [2758]. **biomarker** [2794, 2773, 3431]. **biomarkers** [3735]. **Biomass** [1175, 3558, 1202]. **biomedical** [3641]. **biomolecular** [2133]. **biomolecules** [2075]. **biopolymer** [453, 510, 166]. **Bioreactor** [776, 939, 2152, 2114, 1053, 1183, 1498, 3060, 2051]. **bioreactors** [1653, 2354]. **biosensor** [649, 1813, 1853, 2308, 2250, 1588]. **Biosensors** [828, 880, 934, 901, 1055, 1159, 1849, 1606]. **biparametric** [2761]. **Bipartite** [1025, 818, 810, 3143, 72, 1726, 1000]. **bipolar** [2493]. **bipyramid** [3328]. **bipyramidal** [2027, 2028]. **biquadratic** [3322]. **biradicals** [603, 687, 3462]. **birth** [1686]. **bismuth** [2495, 3612]. **bisphosphonates** [3171]. **Bistable** [2173, 2223, 151]. **Bivariate** [3285]. **Bjerrum** [12]. **blends** [2874, 3001]. **Bloch** [1238]. **Bloch-type** [1238]. **Block** [2833, 3291, 1927, 3286, 366, 2364, 2160, 2161, 3223, 3379, 3440, 242, 3406, 349]. **block-diagonalization** [366, 3379]. **blockage** [2293]. **blocked** [707]. **blocking** [3626]. **Blocks** [916, 2845, 2750]. **blood** [2829]. **blooms** [3121]. **blow** [3193]. **blow-up** [3193]. **blue** [2085]. **bodies** [404, 156]. **Body** [1118, 615, 1877, 3542, 2646, 408, 3091, 2379, 332, 1613, 2174, 1612, 2079, 3251, 2532, 2013, 418, 3555]. **body-frame** [2013]. **Bogdanov** [2577]. **Bohm** [1241]. **Bohr** [1958]. **boiling** [1601]. **Boltzmann** [3599, 3207, 520, 2297]. **Bona** [3673]. **Bond** [928, 831, 819, 844, 876, 3225, 3399, 1971, 2412, 25, 721, 3438, 1617, 446, 1428, 195, 982, 1354, 1235, 1448, 1476, 1452, 1445, 1624, 1623, 1622, 1898, 1830, 1790, 2008, 2087, 2269, 2497, 2877, 683, 3617, 3719, 616, 1788, 2192]. **Bond-Bending** [831]. **bond-breaking** [3438]. **bond-dependency** [1830]. **bond-descriptors** [1354]. **bond-forming** [3438]. **bond-order** [2192]. **bond-projected** [1790]. **Bond-Stretching** [844]. **Bond-Torsion** [819]. **Bonded** [839, 1622]. **Bonding** [3644, 492, 13, 503]. **bondles** [3161]. **Bonds** [909, 885, 1018, 2649, 985, 1269, 1787, 1776, 551, 583, 3718]. **bone** [3171]. **Book** [552, 680]. **Boolean** [2731, 2984, 2983, 3076, 568, 2634, 2858, 2984]. **bootstrapping** [2883]. **boranes** [614]. **Borchardt** [3549]. **bordered** [3149, 3165, 3379]. **Borel** [3657]. **Borel-type** [3657]. **Born** [2148, 886, 2153, 121, 1161]. **Boron** [1010, 3647, 3540, 1763, 1518, 1441]. **boron-containing** [1763]. **boron-nitrogen** [1441]. **Borromean** [403]. **Bose**

[2438, 3091, 1620]. **boson** [2132, 2140, 1060, 2212]. **bosonic** [459, 2212]. **both** [2951]. **bottle** [2593, 2569, 1221, 2950]. **bottom** [1906]. **Botts** [983]. **Bound** [2362, 1132, 1133, 804, 900, 891, 841, 2145, 401, 1266, 787, 1117, 671, 1870, 1467, 3413, 2959, 283, 2564, 2688, 1910, 2575, 2062, 1959, 2639, 1799, 1344, 2703, 232, 489]. **Bound-State** [401, 3413, 2639]. **Boundary** [611, 767, 553, 1062, 2908, 2991, 3543, 3575, 2922, 3361, 3483, 656, 2927, 2943, 3334, 2297, 2346, 2588, 3369, 3601, 3725, 2851, 2855, 2151, 405, 3476, 3147, 3430, 1043, 2954, 2284, 1386, 1781, 2558, 2638, 2637, 2997, 3281, 3327, 3376, 3304, 3495, 3572, 3672, 2335, 2389, 2475, 2618, 3167, 558, 2971, 1644, 2745]. **boundary-driven** [2151]. **bounded** [612, 2062]. **Boundedness** [1896, 628, 1512]. **Bounds** [2508, 2120, 1572, 1025, 3666, 821, 864, 1177, 2479, 1516, 995, 500, 627, 3578, 1262, 1889, 1110, 3341, 1282, 1850, 2222, 2680, 3080, 3029, 437, 737]. **box** [3738, 3392, 2785, 1917, 2820, 1812, 3354]. **Boys** [1091, 936, 2683]. **bracketing** [2400]. **Braess** [3301, 1775]. **braid** [2004]. **brain** [2071, 2651, 2602, 3570]. **branched** [198, 339, 2664, 2625, 535, 342, 1100, 346, 159]. **branching** [1035, 1383, 431, 81, 336, 2578, 626, 2315, 525]. **Brandt** [3346]. **Bratu** [2597, 2975, 3156, 3125, 3297, 3274]. **Bratu-like** [3297]. **Bratu-type** [2597, 2975, 3274]. **Bravais** [672]. **Brazuca** [2728]. **break** [1971]. **break/formation** [1971]. **breakdown** [3701]. **breakdown-free** [3701]. **breaking** [2412, 3337, 2448, 3438, 632, 2285, 1332, 2113]. **breaking/formation** [2412]. **Breast** [1085, 1453, 2431, 2580, 2773]. **breathing** [1477]. **breeding** [3434]. **Bremsstrahlung** [2826]. **bridge** [1581, 1787, 1830, 1776]. **bridges** [30]. **Bridgman** [678]. **brief** [3717]. **Briggs** [3731]. **BROCODE** [3731]. **broken** [3496]. **bromate** [477, 495]. **bromate-ferroin** [477, 495]. **bromoethenes** [734]. **Brownian** [2747, 378, 1410]. **Bruijn** [348]. **Brusselator** [2875, 2944, 3589, 3298, 2359, 2955, 3633, 3584, 1371, 3518, 682, 2988]. **BSA** [2433]. **BSSE** [729]. **BSSE-free** [729]. **BTMEMPR** [2833]. **bubbles** [3150]. **Buckingham** [3251]. **Buckley** [3115]. **Buckminsterfullerene** [429, 458, 388]. **buffer** [3524]. **Building** [916, 2304, 242, 1766, 3634, 2750, 590, 3024]. **bulk** [2800, 3536, 2913, 2521]. **bulk-surface** [2800]. **bullvalene** [396]. **bunch** [2788]. **Burger** [3594]. **Burgers'** [3215, 3573, 3546, 3673, 2082, 3676, 3567, 2529, 2333, 3189]. **Burnside** [893]. **bursting** [3176]. **butadiene** [3001]. **Butanoate** [2990]. **Butlerov** [3436]. **BVPs** [2471].

C

[134, 1485, 192, 1435, 1209, 918, 2387, 2755, 1895, 365, 1565, 1442, 111, 1732]. **C.** [70]. **cactus** [85]. **Cádiz** [3015]. **cage** [3737, 3736, 2735, 365, 525]. **cage-clusters** [525]. **Cages** [849, 846, 268, 1895, 592, 2609]. **Cahn** [3517, 3706]. **calcite** [1531, 1513]. **calcium** [2571, 2069, 3626, 2166]. **calculate** [3078]. **calculated** [1763, 1277, 3004]. **Calculating**

[851, 1107, 2040, 1409, 3138, 2966, 729]. **Calculation** [836, 920, 971, 3626, 2600, 1350, 1456, 1599, 854, 1027, 3188, 199, 561, 2931, 1094, 1607, 2976, 470, 2420, 1312, 1296, 3334, 563, 3418, 2169, 1764, 705, 2081, 1344, 1859, 1722, 601, 203, 2839, 1600]. **Calculations** [1021, 1105, 567, 374, 391, 1096, 318, 2738, 1685, 446, 194, 1872, 2780, 385, 2810]. **Calculus** [778, 2282, 3389, 1244, 20, 3154, 285]. **Calibrated** [536]. **Cambridge** [552]. **Campbell** [217]. **Can** [2578, 1076, 1615, 267, 3492]. **Cancer** [1085, 1139, 1245, 1389, 1453, 1454, 1901, 2072, 2608, 2579, 2580, 2794, 2773, 2702, 3431, 3735, 3460, 2897, 3527]. **candidate** [1906]. **Canonical** [479, 2306, 2279, 1165, 260, 2866, 83, 2474, 1670, 211]. **Cantor** [3076, 3583]. **Cantor-like** [3076]. **capacities** [3058]. **capacitive** [3236, 3070]. **capacity** [2772]. **capped** [994]. **Capra** [1072]. **capsids** [1975]. **capsomeres** [1975]. **capture** [1669, 3132, 3503, 3576, 2988]. **Caputo** [3611]. **car** [214, 614]. **car-parking** [214]. **Carathéodory** [735]. **Carbó** [1757, 1885]. **carbohydrates** [3196]. **Carbon** [1126, 1023, 1188, 1010, 1182, 2375, 892, 2288, 492, 2240, 1680, 2070, 1258, 2074, 438, 1268, 3734, 1318, 1359, 1922, 1813, 3196, 1979, 668, 2167, 2802, 2845, 2918, 2492, 3387, 3448, 1671, 1003, 2163, 589, 268, 2786, 3515, 1428, 2915, 2916, 3550, 592, 3136, 3158, 3505, 3506, 1532, 3254, 2296, 1822, 2640]. **carbonate** [2571, 2069]. **carbonic** [1200]. **carbonyl** [1601]. **carboranes** [126]. **CARDD** [1380, 1372]. **cardiac** [3626, 2973]. **care** [2608, 1396]. **Carlo** [3383, 455, 2947, 3035, 530, 2686, 1587, 1944, 2779, 3622]. **Carlo-stochastic** [455]. **Carrier** [811, 2832, 2587, 459, 696, 697]. **Cartesian** [1246, 2318, 1153, 1859]. **cascaded** [2354]. **Cascades** [1011, 2415, 2679]. **CASE** [2900, 767, 3288, 768, 830, 798, 611, 193, 2225, 1312, 2089, 2681, 2652, 3264, 2864, 553, 3278, 175, 1606, 1662, 2428, 646, 461, 1044, 1054, 1446]. **Cases** [908, 1953]. **Casimir** [3331]. **CASSCF** [2041]. **CASVB** [584]. **cata** [1263]. **cata-condensed** [1263]. **Catacondensed** [1016, 869, 3250, 3148, 3213, 1649]. **catafusenes** [212]. **catalysed** [3393]. **catalysis** [2344, 3609, 2682]. **catalyst** [2964, 2921, 1981]. **catalysts** [2355, 2631, 3533, 2348, 2467, 2561, 2641, 3153, 3256]. **catalytic** [3713, 2927, 2635, 3725, 2974, 2141, 593, 2284, 2116, 2194, 1862]. **catalyzed** [3196, 2819, 1781, 1170, 1248, 3271]. **catastrophe** [3502, 3121]. **catch** [3718]. **catch-bonds** [3718]. **catechol** [1418]. **catenanes** [312]. **caterpillar** [9]. **cationic** [1768]. **caused** [1729]. **causing** [3087]. **caution** [1307]. **cavities** [2758]. **cavity** [2480, 2339]. **Cayley** [2696, 277]. **Cayleyan** [525]. **CB1** [3132]. **CB1-4B** [3132]. **CD** [675]. **CDFT** [3641, 3494]. **CDW** [3132]. **CDW-4B** [3132]. **CE** [1995, 593, 594]. **CEC** [593]. **cell** [2124, 1441, 2790, 1774]. **cell-based** [1774]. **cells** [2254, 2344, 2343, 2905, 2952, 1388, 1689, 1801, 2850, 7, 2687, 2626]. **cellular** [1800, 534, 1767]. **cellulose** [3668]. **cellulose-based** [3668]. **censoring** [3124]. **Center** [920, 854, 758, 1827, 1014, 1167, 1483, 1603, 1737, 1814, 1350, 1456, 1599, 1600, 1482, 946, 1027, 1459, 1460, 1261, 1491, 2987, 3362, 545]. **centered** [197, 3555]. **centers** [1261]. **Central** [975, 360, 1019, 1187, 917,

840, 841, 837, 749, 2010, 1556, 2598, 1388, 2187, 1050, 1045, 1380, 1837]. **Centrality** [1657, 3093]. **centre** [356]. **Centricities** [271]. **centrifugal** [2032, 3178, 3447, 1882, 3444]. **Centroid** [1989, 2103, 2572, 3024]. **cerium** [3590]. **Certain** [872, 139, 140, 2748, 10, 1778, 7, 2707, 2446, 3254, 3133, 463]. **CF** [3342]. **CF-decompositions** [3342]. **CGT** [730]. **CH** [632, 1018]. **Châtelier** [3154, 3154]. **chain** [2705, 918, 414, 3324, 2998, 1035, 1383, 152, 310, 2009, 2235, 2182, 195, 1581, 2306, 307, 2469, 1356, 1310, 1373, 1276, 1561, 1823, 1254, 1317, 1231, 2606, 1789]. **chain-branching** [1383]. **chainlike** [2712]. **Chains** [1128, 751, 843, 1148, 2503, 2636, 3075, 2933, 3585, 1753, 118, 298, 2326, 1363, 2863, 2046, 1186, 1210, 1100, 2609, 30, 2375, 525, 2956, 998, 2783, 1272, 711]. **chains-some** [1363]. **chalcopyrites** [3613]. **challenge** [472]. **Challenges** [794, 3314]. **chamfering** [1072, 1495]. **change** [141, 1408, 3249, 3070]. **changes** [2788, 1969, 1662]. **channel** [1457, 1458, 3590, 3626, 1990]. **channel-blocking** [3626]. **channel-type** [1457, 1458]. **channels** [2240, 2951, 3383, 1269, 1235, 1624, 2008, 2269, 663, 1788]. **Chao** [2872]. **Chaos** [1690, 2398, 2841, 2944, 3157, 2228, 2177, 2199, 2313, 2628, 2615, 3140, 2505, 1373, 1997, 2065]. **Chaotic** [3041, 3711, 2312, 1238]. **Chaoticity** [986]. **CHAp** [2166]. **Chapman** [1360]. **Character** [1169, 146, 3421, 73, 1783]. **Characterisation** [1136, 381]. **Characteristic** [57, 3481, 780, 1753, 107, 170, 1846, 72, 28, 2105, 303, 76, 8, 205, 34, 2428, 300]. **Characteristic-Monomial** [780]. **characteristics** [1908, 3006, 1962, 3536, 2935, 2909, 3356, 3302, 2404, 2954, 1528, 2971, 2914, 2876, 1694]. **Characterization** [1858, 2539, 956, 91, 3445, 1579, 2882, 979, 2874, 1716, 301, 1864, 1221]. **Characterizations** [1143, 3484]. **characterize** [1464, 1463]. **Characterizing** [1173, 991, 1585, 2452, 2080]. **Characters** [859, 348, 1843]. **Charge** [2732, 928, 1167, 1398, 2832, 2951, 3542, 2466, 1770, 2003, 2421, 207, 1603, 1737, 1599, 1600, 1773, 514, 2850, 1365, 2911, 970]. **charge-carrier** [2832]. **Charge-conserving** [1398]. **charge-related** [207]. **charged** [2362, 2448, 2519, 3539]. **charges** [216, 2466, 3419]. **Charles** [18]. **Charlier** [1179, 1793, 2878]. **Chatelier** [2545]. **Chebyshev** [3118, 28, 2583]. **Chem** [1483, 1455]. **ChemDraw** [3625]. **Chemical** [1020, 842, 777, 1493, 857, 2111, 421, 422, 423, 424, 441, 442, 443, 148, 1079, 1034, 3590, 1129, 1107, 1123, 780, 3171, 1499, 340, 1149, 155, 874, 926, 4, 5, 22, 284, 814, 495, 2796, 1269, 1787, 2676, 664, 870, 1056, 1059, 2911, 1061, 1087, 1084, 694, 808, 1208, 3683, 3173, 244, 2814, 2647, 974, 1916, 208, 3401, 975, 2316, 3493, 1676, 2330, 2485, 3022, 2905, 1607, 3577, 1655, 21, 2124, 19, 400, 3287, 1808, 2596, 2329, 598, 2153, 456, 2636, 3226, 3000, 3543, 289, 3660, 1736, 3632, 2291, 3583, 3111, 2516, 1343, 1602]. **chemical** [1472, 2643, 3504, 316, 3564, 2355, 2494, 628, 709, 1686, 3455, 1891, 3711, 539, 606, 3312, 550, 528, 3365, 3311, 3490, 3651, 109, 110, 991, 2870, 1095, 1886, 1887, 1888, 263, 674, 1929, 60, 3627, 420, 407, 46, 1605, 3580, 115, 3342, 3662, 986, 1057, 2066, 2223, 1596, 93, 1842, 2359, 1834, 1920, 2096, 948, 364, 3170,

13, 10, 162, 2970, 3436, 447, 3347, 2955, 3726, 3725, 3681, 134, 2091, 108, 1775, 1242, 2917, 1292, 3692, 2128, 2129, 2342, 2545, 3077, 2864, 3633, 3478, 1895, 3497, 3548, 3608, 92, 719, 2207, 3485, 2285, 2332, 2980, 3244, 1476]. **chemical** [1452, 1445, 1624, 1623, 1622, 1898, 1776, 2087, 436, 3246, 2776, 2707, 3617, 301, 516, 1300, 184, 494, 524, 551, 583, 1647, 2677, 2036, 1331, 2446, 2274, 90, 2246, 3119, 561, 3093, 2486, 2351, 3551, 699, 2729, 131, 272, 3237, 1234, 1407, 1414, 306, 3619, 1974, 3406, 3518, 3611, 3704, 1485, 1825, 160, 3689, 3705, 1610, 2674, 1601, 34, 2838, 3380, 1662, 2525, 3554, 1625, 2881, 430, 484, 64, 65, 3133, 2422, 3670, 3348, 1835, 2698, 3310, 2487, 487, 2520, 551, 1076]. **Chemical/Biochemical** [926]. **Chemically** [3574, 3599, 138, 22, 157, 2036, 2779]. **chemically-powered** [2779]. **chemicals** [2173, 1699]. **Chemist** [913]. **Chemistry** [384, 1085, 942, 3400, 102, 79, 3039, 1683, 1674, 2895, 720, 2696, 3621, 1245, 681, 146, 2560, 391, 3259, 3006, 3130, 3099, 3100, 3557, 1937, 9, 3299, 3325, 3553, 3089, 2245, 3012, 3596, 3005, 585, 256, 609, 667, 53, 54, 58, 134, 3264, 1045, 3131, 3163, 3231, 3242, 3335, 3378, 3480, 3471, 314, 541, 313, 3141, 3061, 3253, 2894, 2244, 2583, 1861, 3513, 3037, 3172, 3186, 3217, 3278, 3364, 3300, 3073, 3152, 3268, 3280, 3349, 3302, 3316, 3586, 68, 77, 246, 270, 3269, 1405, 1036, 1964, 3235, 3063, 1519, 2962, 1872, 3569, 3139, 20, 1774, 2704, 30]. **chemistry** [31, 3370, 3426, 245, 1076, 3162, 3283, 3716, 3092, 2626, 1673, 1923, 1930, 2156, 2328, 2476, 2754, 3160, 3187, 540, 3044, 3592, 3724, 3407, 3064, 3134, 2766, 3511, 3097]. **chemistry-related** [1930, 2156]. **chemists** [1396]. **chemomechanical** [704]. **Chemostat** [1022, 1024, 2168, 1007, 1515, 1584, 1504, 1356, 1310, 1373, 1276, 1512, 1583, 1195, 1240, 1594, 1254, 1317, 1374, 1231, 1340, 1301, 2610, 3597, 2165]. **chemostat-type** [1584]. **chemotherapy** [3098]. **Chen** [2872, 1978]. **Chidsey** [2261]. **Chinese** [3324]. **Chiral** [3337, 2012, 1420, 110, 2243, 404, 620, 2681, 387, 371, 439, 464, 490, 2285, 1694, 461, 1380]. **Chirality** [130, 3396, 904, 4, 29, 1072, 1138, 3623, 1108, 1089, 144, 3710, 3694, 143, 486, 2598, 629, 2209, 2027, 2584, 2585, 383, 394, 2543, 5, 158, 604, 454, 493, 1319, 1380, 582, 571, 1304, 368, 432, 369, 2027, 2451]. **Chiralization** [22]. **chloride** [1827]. **chloronaphthalenes** [2137]. **chlorophyll** [2617]. **choice** [1282, 1850]. **choosing** [2567]. **Christoffel** [135]. **chromatogram** [2226]. **chromatography** [2976]. **chromen** [1976]. **Chromophores** [248]. **chronoamperometric** [1957]. **chronoamperometry** [1334, 1377, 1714, 1715]. **chronopotentiometry** [513, 514, 593]. **chrysin** [3460]. **Chun** [2501, 2456]. **CI** [521, 1488, 1569, 1903, 2627]. **circles** [149]. **circuit** [107, 303, 185]. **Circuits** [786, 3338, 431]. **circulant** [2852, 2531]. **Circular** [767, 3738, 611, 706, 553, 2565]. **circumscribed** [2613]. **cis** [2539, 2961, 2711]. **cis-** [2539, 2948]. **Citrate** [3431]. **Clar** [2823, 15, 2217, 375, 2326, 1073, 818, 3214, 998, 1117, 1732]. **clarification** [2545]. **Class** [907, 911, 1172, 1224, 3587, 1896, 3117, 2249, 3372, 2812, 3535, 657, 3170, 2346, 1194, 1303, 3262, 1045, 2639, 559, 235, 3119, 2031, 2638, 2637, 2997, 3281, 3304, 3495, 3572, 3672, 2581, 3167, 3351, 2813, 973, 1311, 3028].

classes [3338, 3168, 61, 3439, 2892, 3433, 357, 1828, 449, 1913]. **classic** [1878, 20]. **Classical** [951, 1286, 932, 1116, 2590, 3542, 467, 2386, 416, 1881, 3137, 3443, 1241, 610, 2242, 1994, 2247, 1194, 1303, 427, 2198, 219, 3058, 2267, 245, 3597, 2743]. **Classification** [1646, 2039, 387, 212, 2728, 93, 427, 371, 578, 3024, 3194, 112, 236, 2273]. **classified** [213]. **Classifying** [316]. **Clebsch** [3637, 97]. **Clifford** [3169]. **clinical** [1661, 1389, 2255, 3570]. **clock** [477, 3422, 664, 3704]. **Close** [3261, 2316, 3438]. **Close-to-zero** [3261]. **close-up** [3438]. **Closed** [887, 2221, 2711, 601, 1357, 3715, 798, 3155, 709, 1665, 1366, 608, 586, 228, 485, 2073, 2295, 2489, 548, 1349, 235, 1993]. **Closed-Form** [887, 601, 3715]. **closed-shell** [3155]. **closer** [2055]. **cloth** [2786]. **cloud** [1915]. **clouds** [3432, 1989, 2058, 1440]. **Cluj** [1419]. **Cluster** [529, 1134, 902, 876, 1942, 220, 3641, 1902, 3417, 1994, 94, 2788, 2469, 2708, 533, 322]. **clustered** [3445]. **Clustering** [1079, 1095, 3201, 166, 2081]. **clusterized** [1675]. **clusters** [2653, 2906, 2771, 2290, 1555, 2918, 3035, 2570, 13, 2972, 1685, 3146, 3541, 242, 277, 525]. **CMB** [1933, 1927, 2158]. **CML** [3041]. **CMMSE** [1684, 2886, 3401, 2887, 3099, 3043, 3429, 3017, 2890, 3434, 3027, 3675, 2889, 3359, 3102, 2476, 3097, 1688]. **CMMSE-09** [1688]. **CMMSE-17** [2887]. **CMMSE-2009** [1684]. **CMMSE-2014** [2476]. **CMMSE-2019** [3099]. **CMMSE2017** [2892]. **CNTs** [3506, 2102]. **CNTs-based** [2102]. **CO** [1069, 1069, 2641, 2924]. **coarse** [2075, 2710, 3334]. **coarse-grained** [2710, 3334]. **Coating** [2755, 2433, 1550]. **cocoa** [3434]. **code** [1213]. **Codes** [826, 3161, 2053, 1894, 1473]. **codification** [1380]. **Codimension** [3455]. **Codimension-2** [3455]. **Coding** [267, 260, 3626]. **codon** [1364]. **codonically** [2257]. **codons** [1273]. **Coefficient** [1469, 1024, 1369, 2873, 528, 407, 1714, 1715, 3593, 2531, 2717, 378, 1504, 558, 1551]. **coefficient-theorem** [407]. **Coefficients** [768, 870, 3637, 2249, 379, 3544, 60, 457, 1710, 1994, 28, 944, 97, 1045, 2896, 3227, 1764, 572, 3058, 2265, 2442, 2601, 2699, 2931, 106, 3212]. **coexist** [3492]. **coexistence** [2267]. **coffee** [3429]. **coherence** [615]. **coherence-transfer** [615]. **coherent** [718, 415, 1598, 2131, 2365, 2275, 2552, 2713, 3289, 3566]. **coin** [2396]. **coincident** [644]. **collapse** [339, 2093]. **collapses** [2614]. **collapsing** [198]. **Collatz** [3305]. **collection** [3621, 1402]. **Collective** [2106, 2443, 2649, 2617]. **collinear** [675, 3087, 3547]. **collision** [2875, 3599, 1851, 3733, 1766]. **Collisional** [2092]. **collisions** [1669, 1668, 2951, 3442, 3441, 3542]. **Collocation** [3517, 3528, 3633, 3513, 3156, 3125, 3304, 3572, 3297, 3239, 3197, 3584, 3274, 1358, 2997]. **Collocation-based** [3517]. **colony** [3530]. **color** [2309, 1314]. **Colored** [929, 378]. **coloring** [3071]. **colorings** [2928, 2981, 3085, 3710, 3694, 2020]. **column** [2058, 2272]. **Combination** [1065, 1145, 3567, 2044, 2036, 1573, 1732]. **Combinatorial** [910, 2928, 3204, 3709, 262, 820, 991, 1154, 1229, 2491, 118, 2309, 2906, 3201, 535, 1586, 1965, 3340, 540, 1187]. **combinatorial/geometric** [1586, 1965]. **combinatoric** [636, 701]. **Combinatorics**

[2653, 3710, 3700, 780, 540, 2981, 3085, 3560, 3740]. **Combined** [1151, 1604, 2038, 1455, 2373, 2748, 2496, 2298, 2299, 2371, 2372, 2907, 2936, 3145, 3043, 1050, 1366, 1595, 542, 2749]. **combined-permutation** [2907, 2936, 3145]. **combines** [3098]. **Combining** [2193, 1939, 3440]. **Combustion** [1035, 907, 2189, 955, 1383, 2045, 2744, 2436]. **Comment** [2785, 1978, 2872, 3010, 3299, 3312, 3313, 3447, 920, 1483, 153, 2313, 1131, 829, 1027, 1455, 1485, 122, 754]. **Comments** [1162, 1163, 3724]. **Common** [244]. **Communication** [1448, 1436, 1452, 1445, 1624, 1623, 1788]. **Communication-theory** [1448, 1452]. **Communications** [2269, 1629, 1787, 1802, 2270, 2345, 2432]. **commutative** [1804]. **Commuting** [866]. **Compact** [3362, 442, 443, 3483, 2694, 3459, 3559, 3509, 3603, 1655]. **Comparability** [105]. **Comparative** [3448, 1377, 2333, 3209, 3537, 3647, 1334, 3607, 1667, 3058]. **compared** [3425]. **Comparison** [886, 752, 1072, 2222, 214, 2705, 2920, 351, 2131, 1602, 275, 624, 1702, 2169, 1513, 3675, 3359, 2076, 1000, 978, 128]. **comparisons** [1989]. **compartmental** [2017, 2018, 2368, 2369, 3351]. **Compatible** [811]. **competing** [2238]. **Competition** [1053, 1374, 1183, 1584]. **Competitive** [875, 2610, 2045, 2744, 1564, 2822]. **competitor** [1053]. **Complementarity** [897]. **Complete** [400, 212, 1014, 3270, 3336, 855, 3163, 1976, 433, 273, 1205, 1321, 1284, 1338, 1385, 1468, 1475, 1604, 3005, 3131, 195, 1221, 3092, 2971]. **Completely** [2203, 423, 1332]. **completeness** [4]. **completion** [210]. **Complex** [1032, 2980, 2667, 1240, 2520, 3409, 975, 2842, 1607, 2082, 3487, 1814, 1057, 2091, 2690, 1307, 2246, 2031, 3138, 1234, 695, 1825, 3236, 116, 1278]. **complex-balanced** [2246]. **complexes** [3583, 88, 2936, 3418, 2575, 2252, 2753, 2948, 2992, 1551]. **complexing** [3589]. **Complexity** [19, 2823, 2465, 3298, 3529, 1709, 1755, 1219, 1702, 2030, 3049, 3416, 3425, 1042, 3119, 3414, 1376, 1563, 1558]. **complexity-based** [1558]. **Compliance** [1349]. **component** [2920, 1578, 2748, 1214, 1604, 2035, 1909, 2327, 3584, 2749, 1285]. **Components** [818, 2773, 3431, 744, 1910, 513, 1776, 2661, 1611]. **composed** [2973]. **composite** [2479, 3374, 2212]. **composition** [1887, 2269, 970, 2706]. **compositions** [2653, 2066]. **compound** [3124, 2911]. **Compounds** [872, 171, 2341, 25, 1457, 1458, 991, 2027, 2028, 3145, 263, 13, 162, 3478, 92, 3719, 2263, 3119, 1069, 670, 2197, 1293]. **Compressing** [3421]. **compression** [3506]. **comprising** [2167, 3688]. **Computation** [1113, 756, 792, 2817, 953, 839, 782, 2721, 3555, 3371, 3128, 2528, 3053, 1226, 3233, 135, 186, 2496, 3010, 2742, 3544, 265, 1394, 1336, 1785, 150, 2704, 1899, 1839]. **Computational** [2981, 3085, 1055, 1159, 2964, 3390, 1509, 1775, 1606, 959, 3629, 3015, 3642, 2929, 2544, 1683, 1762, 2812, 24, 1213, 3079, 2359, 3594, 84, 2955, 3640, 2770, 2897, 3037, 3654, 2511, 3495, 3672, 2753, 2948, 2581, 3619, 710, 3638, 1673, 1923, 2328, 2476, 2754, 440, 1688]. **computationally** [2734]. **computations** [2688, 554]. **compute** [39, 3177]. **computed** [3625]. **Computer** [171, 260, 25,

1003, 1032, 2166, 2506, 1930, 193, 462, 986, 530, 1194, 1303, 2055, 1100, 1409]. **Computer-aided** [171]. **Computer-assisted** [25]. **Computing** [2866, 531, 1472, 895, 2011, 1140, 76, 1616, 810, 3375, 3701, 1934]. **comrade** [3701]. **concatenation** [3076]. **concealed** [82, 274]. **concentrate** [1932]. **Concentration** [2502, 2095, 1995, 3011, 2849, 1768, 1704, 1999, 1824, 989, 1195, 1733, 1193, 2422, 3492]. **concentrations** [2492, 2369, 3136, 2512]. **concentric** [1817]. **Concept** [1173, 1443, 2111, 488, 124, 604, 92, 98, 223, 731]. **Concepts** [850, 102, 789, 80, 2358, 333, 449, 2865]. **conceptual** [3458]. **concerned** [2111]. **Concerning** [866, 1298, 711]. **Concise** [870]. **concurrent** [3544]. **condensates** [2438, 3091]. **condensation** [3580, 712]. **Condensed** [3719, 2613, 1263]. **Condensed-to-bond** [3719]. **Condition** [905, 3489, 3135, 51, 989, 3677, 1644, 2745]. **conditional** [1790]. **conditionally** [3335]. **Conditions** [1062, 1628, 2757, 3108, 707, 3575, 3483, 656, 1334, 3334, 2438, 2297, 2970, 3725, 333, 449, 2904, 1943, 372, 405, 235, 1043, 2475, 2618, 1238, 1819, 1541, 2195, 2428, 1938]. **Condon** [659, 608, 3078]. **Conductance** [781]. **conducting** [1212, 1824]. **conduction** [425]. **conductive** [2750]. **Conductivities** [2495]. **conductivity** [2479, 2233]. **Conference** [959, 3015, 3017]. **confidence** [536]. **Configuration** [785, 1948, 2358, 2452, 279, 2169, 2184, 315, 2269, 730, 326, 463, 2706]. **Configurational** [253, 1721, 434, 159]. **Configurations** [263, 1817, 99, 1398]. **Confined** [762, 3392, 2276, 3049, 3476, 3469, 2818, 950, 1100, 2630]. **Confinement** [822, 877, 2187, 2183]. **confirmative** [2749]. **confluent** [36, 2639]. **conformal** [3162]. **conformation** [962, 2235, 2182, 1497, 1719, 565]. **Conformational** [1187, 2314, 2153, 3294, 1388, 202, 155, 191, 2788, 636, 701, 67]. **conformationally** [100]. **conformations** [316, 341, 1261]. **conformers** [445, 2753, 2948, 517]. **confused** [1688]. **Congress** [384]. **Conic** [1188]. **conical** [2539]. **conicality** [2160]. **Conjecture** [884, 883, 2573, 855, 949, 957, 1632, 1735, 1860, 141, 2603, 2670, 2731, 2782, 3071, 3520, 137, 229, 1298, 373, 2716, 3305, 2076, 2634]. **conjectures** [3375, 336, 555]. **conjoining** [3540]. **conjugacy** [2812, 2659, 1834, 1920, 2657]. **conjugate** [3539]. **Conjugated** [786, 1023, 1088, 1031, 933, 868, 978, 2496, 1265, 153, 252, 643, 1189, 172, 70, 1332, 3719, 185, 73]. **conjugated-circuit** [185]. **Connect** [1090]. **connected** [1163, 1313, 1111, 2821]. **connecting** [377]. **Connection** [932, 1308, 2082, 1805, 3004, 1327, 1648, 95, 1967, 2652]. **Connections** [844, 1058, 1363]. **Connectivity** [849, 3225, 3399, 3183, 3531, 1728, 1631, 1281, 162, 1506, 1768, 1716, 1228, 3554, 1720, 1649, 1560, 1566, 1590]. **consecutive** [2494, 2541, 2499, 2725, 1319]. **consequence** [2121]. **Consequences** [857, 2983, 118, 1613, 3246]. **Conservation** [3706, 3151, 3016, 3115, 1184, 3020, 3257, 2486, 3667, 3112, 2487]. **conserving** [1398]. **considerably** [3431]. **consideration** [2802]. **considerations** [202, 1741, 2674, 729]. **consistency** [413]. **consistent**

[2463, 1105, 2742, 243, 635, 242, 1161]. **consisting** [2703, 694]. **Constancy** [1879, 2900]. **Constant** [3474, 873, 2827, 3122, 3301, 1320, 1283, 2199, 2628, 1237, 2505, 3227, 2721, 1670, 2441, 2440]. **Constantin** [735]. **Constants** [1135, 1926, 3303, 2355, 2193, 1296, 1503, 1954, 2515, 1851, 3423, 2799, 2023, 1542]. **constitutional** [53, 54, 3462, 3093]. **constrained** [2672, 2473]. **constraint** [1184]. **Constraints** [1348, 2836, 1150]. **Construct** [778]. **constructed** [2700]. **Constructing** [1971, 2412, 2788, 3634, 3043, 1601]. **Construction** [1875, 806, 2098, 1527, 2443, 3241, 2435, 2468, 2728, 2985, 2275, 2552, 2108, 1500, 1845]. **constructive** [1886, 1887, 1888, 2427, 221]. **consumption** [664]. **contact** [3247]. **Containing** [825, 2341, 1763, 1975, 2327, 1044, 1054]. **contains** [1253]. **contamination** [1545]. **contemporary** [2089, 2090]. **content** [2263, 3119]. **context** [1041, 322]. **continua** [948, 692]. **continuation** [2903]. **continued** [1591]. **continuity** [1236, 2497, 2619]. **Continuous** [1020, 770, 653, 2636, 2152, 2114, 3661, 120, 571, 699, 1520, 2051, 2354, 987]. **continuous-time** [2636]. **Continuously** [802, 738]. **Continuum** [246, 401, 2951, 595, 2294, 2793, 3387, 1874, 960, 958, 2521]. **Contois** [2152]. **contorted** [2134]. **contour** [990, 43, 70]. **contour-integral** [70]. **Contraction** [324]. **contribution** [2608, 406, 1722, 1583]. **contributions** [408]. **Control** [794, 776, 939, 2658, 2453, 2330, 3022, 1800, 367, 2739, 416, 500, 2841, 2944, 3157, 2292, 2473, 1686, 3711, 2517, 1552, 2567, 1538, 1405, 2353, 2262, 1335, 3069, 3635, 1857, 3348, 3657, 1658]. **Controllability** [2186, 2643, 605]. **Controlled** [1013, 757, 500, 3060]. **controller** [3348]. **controlling** [1849]. **convection** [3106, 3565, 1225, 1316, 1190, 1710, 3712, 3607, 3397, 3595, 2416]. **convection-diffusion** [3565, 3595]. **convective** [2635, 2484]. **conventional** [2967, 2027, 1096, 1705, 1639, 214]. **Convergence** [2757, 3602, 140, 3417, 102, 758, 3116, 2647, 2759, 2895, 3031, 3114, 2901, 2995, 564, 1049, 2160, 3113, 3110, 2763, 2904, 3107, 2645, 2796, 1785, 533, 3672, 556, 2749, 2428, 2880, 3014, 3510]. **Convergent** [1105, 3404, 3681, 3197]. **converging** [2974]. **Conversion** [901, 1853, 344]. **converting** [195]. **Convex** [1071, 598, 597, 1586, 3069]. **Convexity** [937, 44, 7]. **convolution** [2449, 516]. **cooling** [1924]. **Cooper** [3498]. **Cooperative** [1018]. **cooperativity** [2311]. **Coordinate** [920, 854, 1027, 2712, 142, 2196, 135, 1472, 1205, 1284, 1338, 1385, 1468, 2710, 3334, 1350, 1456, 1599, 1600, 33, 2661, 452, 1859, 160]. **coordinated** [3618]. **Coordinates** [941, 2498, 2188, 135, 1246, 1198, 1914, 279, 2013, 219, 1491, 1488, 1569, 2627, 1969, 3211, 2792]. **coordination** [381]. **Cope** [396]. **copolymer** [1413, 3583, 1682]. **copolymers** [153, 2599, 392]. **CORAL** [1746, 2197]. **corazulenic** [1422]. **Core** [943, 1300, 1496, 3418]. **core-ionization** [1496]. **Coriolis** [2968]. **Corner** [1827]. **cornerstone** [2741]. **corona** [3219]. **coronoid** [295]. **Coronoids** [2622]. **corral** [2097]. **corrected** [2708, 3488]. **correcting** [3066]. **Correction** [3737, 3442, 3100, 3678, 3563, 3605, 3620, 3581, 3591, 3368, 2916, 2810, 3716, 3014]. **corrections** [728, 3382]. **Corrector** [1099, 2524, 2472, 3673, 2213, 967, 2380, 2930].

Correlated [1612, 830, 2130, 1659, 1769, 1909, 96, 1966, 2839]. **Correlation** [940, 1585, 992, 2117, 3123, 2148, 1490, 87, 6, 3273, 655, 2384, 2652, 3547, 317, 3190, 3191, 3192, 2385, 1069, 3625, 506, 730, 3622, 961, 2133, 1688, 109]. **Correlations** [1305, 1884, 3182, 2019, 686]. **correspondence** [104]. **Corresponding** [933, 303, 1201]. **corrupted** [2431]. **Corzo** [2785]. **Coset** [929, 1154, 109, 110, 161]. **Cosets** [929, 1154]. **Cosine** [1132, 1737, 2780, 2810]. **Cosine-Screened** [1132]. **Cosines** [827, 1915]. **CoSMEP** [2203]. **Cost** [3610, 3400, 2544, 3493, 3504, 3464, 2786, 3480, 3471, 3586, 2511, 3426, 3592, 3724]. **Cost-Effective** [3400, 3471, 3426]. **cost-efficient** [3464, 3592, 3724]. **Cost-reduction** [3610]. **Costa** [3015]. **Cotangent** [835]. **Cotes** [1956, 1357, 1993]. **Coulomb** [1940, 1396, 2287, 2466, 3232, 1156, 3402, 1665, 919, 971, 1050, 1659, 1769, 2042, 1132, 1133, 228, 3308, 2605, 3425, 2668, 1635, 401, 3545, 758, 3715, 1742, 2083]. **Coulombic** [3010, 2817]. **Coulson** [209, 18, 952, 1051, 103, 1752, 70, 285]. **Count** [896, 1128, 1417, 2266, 225, 1000, 1732]. **counterexample** [2326]. **Counterexamples** [2063, 373]. **counterions** [2235, 2182]. **Counting** [2414, 2066, 1403, 1819, 161, 237, 350, 349]. **counts** [264, 1390, 2134, 153, 2088, 2100]. **Coupled** [3206, 902, 1981, 3195, 974, 2343, 3205, 2124, 400, 501, 502, 2418, 1690, 1679, 736, 2927, 2245, 1477, 3726, 2228, 2177, 2199, 2313, 2559, 2628, 2615, 3140, 3159, 2505, 3008, 2507, 2708, 590, 533, 2284, 1519, 3595, 2232, 3467, 3518, 3556, 3546, 2395, 1997, 2065, 2792]. **Coupled-Cluster** [902, 533]. **coupled-rotors** [3195]. **Coupling** [572, 2314, 1743, 3041, 2199, 2628, 2505, 3541, 1349, 1734, 1629, 436, 2229, 2968, 2912, 2441, 2440, 1620, 1727]. **course** [3432, 1577]. **Covalent** [3484, 981, 3371, 35]. **Covalently** [839]. **covariance** [30, 31]. **coverable** [295]. **coverings** [342]. **COVID** [3631, 3629, 3646]. **COVID-19** [3631, 3629, 3646]. **covolume** [3501]. **Craciun** [1485]. **created** [1823]. **Creatine** [798]. **Cremer** [1914]. **Criteria** [3093, 1795, 190, 3047]. **Criterion** [752, 564, 3658, 2001, 3311, 3651, 2260, 162]. **Critical** [3392, 14, 747, 1628, 2478, 3035, 345, 1768, 2267, 3169, 1803, 1967, 1727]. **Cross** [3576, 756, 768, 3132, 3685, 3424, 1260, 1823, 349, 3690]. **cross-diffusion** [1823, 3690]. **cross-section** [1260]. **Cross-Term** [768]. **Cross-Validated** [756]. **crossing** [2408, 2533]. **crossings** [1945]. **crosslinked** [2693]. **crosslinking** [2115]. **Crossover** [2212, 2268]. **crowded** [3061]. **Crowley** [2165]. **crystal** [3417, 2721, 3276, 3505]. **crystalline** [981, 1493, 1918]. **Crystallization** [774, 1924]. **crystallographic** [428]. **crystals** [595, 3334, 3035, 1685, 3537]. **CTI** [207]. **Cu** [498, 2750, 1547]. **Cu-wire-mediated** [2750]. **Cube** [1010, 1237]. **cubes** [3053]. **Cubic** [910, 1104, 793, 1806, 2053, 3607, 3726, 1425, 3508, 419, 508, 436, 3357, 518, 3555, 1726, 3505, 1573, 3650]. **cuboctahedron** [284]. **culture** [1658, 987]. **Cumulants** [1113]. **cured** [2489, 2515]. **Current** [148, 2264, 1316, 1190, 513, 2488, 1824, 1862, 3642]. **current-concentration** [1824]. **currents** [1003, 1428, 2084]. **curvature** [668, 2502]. **Curve** [752, 1021, 761, 3385, 3455, 201, 1092, 447, 658, 1717]. **Curved**

[380, 479, 382]. **Curves** [1108, 2504, 2421, 113, 46, 2267, 35, 1304, 1339]. **Curvilinear** [941, 2013]. **cusp** [3489]. **cusps** [496]. **Cut** [766, 2663, 3482, 2768]. **Cuts** [1140, 1333, 1627]. **cuttings** [2157]. **cyano** [1293]. **cyano-compounds** [1293]. **cyanobacteria** [3121]. **Cycle** [780, 929, 843, 61, 633, 3287, 3448, 109, 2049, 2299, 2372, 2585, 2546, 2729, 2584]. **cycles** [3179, 1554, 2496, 1225, 120, 458, 1832, 1474, 2159, 1319, 372, 699, 306, 1625, 987, 1387]. **Cyclic** [901, 1128, 1333, 1627, 1932, 25, 2777, 2785, 1917, 2592, 3062, 3593, 3702, 172, 514, 593, 3093, 2257, 2692]. **Cyclical** [849, 1228]. **Cyclicity** [781]. **cyclo** [1978, 1507, 998]. **cyclo-polyphenacenes** [1978, 1507, 998]. **cyclobutane** [1585]. **Cyclobutanes** [1134]. **Cyclofusene** [909, 1071, 985, 1111, 1275, 1586]. **cyclofusenes** [1313]. **cyclohexane** [2805]. **Cyclooxygenase** [3194]. **Cyclooxygenase-2** [3194]. **cyclopropyl** [2041]. **cylinder** [2374]. **cylinders** [2672, 357]. **Cylindrical** [767, 611, 2569, 553, 2471]. **Cytosolic** [1067]. **cytotoxic** [1801]. **Cyvin** [132, 373].

D [1978, 2424, 1444, 2872, 1372, 1592, 683, 672, 2968, 3106, 2928, 2981, 3009, 2755, 2555, 2923, 2216, 1286, 3036, 1092, 2480, 1749, 2025, 2339, 2548, 1141, 1075, 1380, 2791, 1043, 2857, 1864, 250, 2273, 2061, 2968, 2743, 183]. **D-chiral** [1380]. **D-dimensional** [2424]. **D-dynamic** [2273]. **D-hypercubes** [2928, 2981]. **D-MORPH** [1749, 2025, 2548]. **D-parabolic** [3106]. **d-space** [183]. **D2h** [1155]. **D2h-symmetries** [1155]. **DAEM** [3059, 1202, 1175]. **damaged** [2343]. **damped** [2842, 2896, 3151]. **Dancoff** [2445]. **Darboux** [2360, 1837]. **Darcy** [2484]. **Data** [890, 1175, 1079, 766, 789, 921, 3582, 1094, 2608, 2579, 2602, 2794, 1243, 3634, 3258, 3216, 539, 2069, 1707, 1957, 1710, 3446, 200, 1749, 2025, 2864, 1717, 3001, 3046, 2707, 3422, 1335, 3659, 1821, 2022, 2258, 3317]. **Databases** [789, 1095, 1399]. **datamining** [3627]. **datasets** [3024]. **DD** [1339]. **DD-Curves** [1339]. **DDRP** [451]. **de-** [3634]. **de-excitations** [1939]. **deactivation** [3258]. **deal** [350]. **DeAngelis** [1356, 1374, 1340]. **death** [2051]. **decay** [990, 3247, 539, 3411, 2402, 436, 2404, 2987]. **Deciphering** [1213]. **decision** [3628]. **Decisive** [1139]. **Decomposition** [752, 1700, 2332, 3258, 2492, 3034, 2379, 2707, 2284, 247, 2335, 2192, 2340]. **decompositions** [3587, 2756, 3342, 1427, 2769, 3649]. **deconstruction** [1792]. **deconvolution** [997]. **decorated** [3326]. **decoupled** [2126]. **decrease** [3087]. **decreased** [3431]. **Deduction** [984]. **deductions** [1198]. **Defect** [822, 3345, 2376]. **defect-induced** [2376]. **defective** [3568]. **defects** [2686]. **Deficiency** [3286, 2939, 1089, 2249, 1905, 582, 1969, 2657]. **deficiency-one** [2249]. **Deficit** [781]. **define** [3255]. **defined** [3432, 1952, 2665, 3071, 2982, 2415, 2675, 413]. **Defines** [905]. **defining** [3634]. **Definition** [857, 1598, 456, 2153, 2136, 581, 2280, 577]. **definitions** [2443, 1773, 2799]. **deformed** [954, 2879, 2445, 2227, 2132, 3203, 1614]. **deg** [3522]. **Degeneracy** [352, 1075, 207, 6, 234, 2214, 1721]. **Degenerate** [908, 259, 3699, 340, 162, 2497]. **Degradation** [2250, 2787]. **degree**

[2663, 144, 612, 3007, 947, 5, 1470, 156, 3461, 3521, 3684, 3032, 1500, 1845, 3615, 2821, 1593, 369]. **Degrees** [1090, 1948, 2578, 1571]. **dehydration** [1534]. **Dehydrogenase** [798, 3196]. **dehydrogenase/laccase** [3196]. **deionization** [2830, 3236, 3070]. **Delay** [903, 1857, 3598, 3404, 2168, 1564, 1584, 1725, 3695, 3635]. **delayed** [1515, 3055, 2416, 3597]. **delays** [2165, 3725]. **delivery** [3060]. **delocalization** [2785, 1917, 2097]. **delocalized** [2986]. **Delta** [884, 685, 3734, 1792]. **Democratic** [811, 615, 697]. **Democratic-Recoupling** [811]. **Dendrimer** [3356]. **dendrimers** [1719, 565]. **dendrons** [1719]. **Deng** [1978, 3126, 2099, 2145]. **dense** [1616]. **densit** [355]. **Densities** [801, 1167, 401, 830, 722, 2976, 2448, 1603, 1737, 2324, 3366, 465, 583, 1838, 737, 133, 3452]. **Density** [861, 1113, 1179, 927, 1105, 822, 1859, 2180, 2130, 141, 2203, 2202, 598, 1369, 1287, 1288, 1289, 1744, 1805, 2196, 2103, 2136, 2176, 2383, 2466, 1869, 3489, 3233, 338, 3479, 1384, 304, 2187, 2021, 1096, 3417, 547, 1747, 2324, 504, 228, 276, 747, 1599, 1600, 852, 1773, 1966, 3547, 465, 1398, 1440, 1968, 2449, 3654, 2094, 2730, 3416, 1612, 3719, 1535, 2660, 601, 324, 961, 1756, 440]. **Density-based** [1105]. **density-functional** [3547]. **deoxyribonucleic** [2685]. **Dependence** [1256, 876, 253, 1236, 2732, 2095, 2249, 1243, 191, 1645, 2008, 683, 159, 2442]. **dependencies** [3492]. **dependency** [1830]. **Dependent** [888, 887, 1556, 1494, 3565, 3323, 2873, 3383, 2408, 2533, 2035, 1741, 1247, 3397, 2169, 2184, 2419, 2896, 2281, 2056, 3354, 3388, 3476, 1678, 2618, 2512, 654, 3266, 2604, 1165, 2699, 389, 390, 1044]. **depending** [1395, 1670]. **depletion** [2562]. **Derivation** [608, 2180, 319, 659, 2017, 511, 2306, 2365, 1851, 1541]. **derivations** [678]. **Derivative** [3205, 3206, 3500, 685, 1745, 1871, 2392, 2908, 2647, 2995, 3117, 2920, 2967, 3083, 3288, 3292, 3431, 3538, 3604, 3570, 3720, 3697, 3735, 3543, 3564, 2283, 2893, 3674, 1671, 201, 2633, 3026, 3253, 2903, 3364, 2381, 2930, 3266, 3611, 1500, 1845, 3491, 2835, 3030, 3407, 2697, 2853]. **derivative-modified** [1671]. **Derivatives** [820, 872, 1754, 1798, 2060, 2029, 2118, 2178, 2253, 2410, 2322, 2544, 2524, 2549, 2472, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 2908, 1559, 2842, 2809, 2734, 2746, 3565, 2587, 991, 1585, 2048, 2049, 1050, 1246, 1874, 2566, 1840, 3242, 3378, 3471, 3460, 2733, 3172, 3186, 3243, 3278, 2867, 1430, 2507, 2511, 1904, 2098, 2317, 2370, 2455, 2607, 3370, 3426, 3160, 3187, 3218, 2648, 2594]. **derive** [3730, 279]. **Derived** [6, 3624, 3145, 1894, 547, 1716, 1069, 1988, 1076, 459, 555, 260]. **Desargues** [2906]. **describe** [2357, 1918, 2850]. **described** [2136, 3337]. **describing** [1808, 1234]. **Description** [570, 870, 1208, 718, 2254, 2344, 2504, 564, 1989, 2188, 2649, 3071, 2307, 1421, 3387, 2382, 2274, 1408]. **descriptions** [248]. **Descriptor** [848, 3499, 2457, 3563, 3605, 3620, 3581, 3591, 3562, 3534, 1440, 3719, 2233, 1708]. **Descriptors** [1070, 1123, 2273, 3686, 3737, 3736, 1763, 1351, 1615, 2555, 3627, 427, 1380,

1372, 3620, 3581, 3591, 3534, 1354, 1476, 1623, 1898, 2008, 2269, 2345, 2432, 2551, 2527, 2619, 3623, 163, 3209, 2607, 1788, 3068, 1565, 1551, 1621, 2340]. **Design** [1932, 2862, 305, 2411, 510, 2193, 1497, 1426, 2056, 2911, 3348]. **designed** [3601]. **designing** [2609, 2655]. **designs** [3675]. **desired** [1582]. **desorption** [1069, 2194]. **destroyed** [2327]. **Desymmetrization** [144]. **detachment** [2521]. **detailed** [1990, 131, 1825, 1544, 2520]. **Details** [126]. **Detecting** [1933, 131, 2158]. **Detection** [1085, 2072, 1634]. **deterioration** [2430]. **Determinable** [525]. **Determinacy** [614]. **determinant** [113, 3202, 2807, 3381, 3477, 2251, 2953, 522, 482]. **determinants** [3701, 3062, 3165, 3223, 3379, 3464, 2852]. **Determination** [3384, 1175, 3318, 1187, 2482, 1538, 3284, 1362, 1277, 1770, 1957, 1447, 1047, 1842, 3306, 2864, 2295, 2515, 683, 2799, 3169, 2912, 64]. **Determine** [772, 2351, 2265, 2442, 2601]. **determined** [2939, 278, 251, 2706]. **Determining** [890, 2069, 2059, 1662, 2805, 1932, 2187, 71, 1790, 2108, 2157, 1335, 2650]. **Deterministic** [774, 1686]. **detour** [1581]. **detoxification** [3082]. **Deuterated** [734]. **deuterium** [192]. **developed** [3145]. **Development** [2752, 2655, 2632, 1526, 3084, 623, 426, 2776, 763, 764]. **developments** [1508, 85]. **Deviation** [1729, 1538, 2565]. **deviations** [1792]. **device** [3348]. **devices** [456, 1767]. **Devil** [703]. **devising** [6]. **Dewar** [3734, 2907]. **dewetting** [2694]. **DF** [2058]. **DFT** [2094, 2538, 3489, 3458]. **Di-Substitution** [872]. **Diabatic** [886, 898, 974, 1971, 2412]. **diagnosis** [81]. **diagnostic** [2829, 2255, 2651]. **diagnostics** [1139, 1245, 1389, 1453, 1454, 1901, 2579, 2580, 2602, 2702, 3292, 3720]. **Diagonal** [865, 1369, 598, 2139, 2251, 1612]. **Diagonalization** [1081, 366, 2364, 3223, 3379]. **diagonally** [3224]. **Diagrammatic** [902]. **Diagrammatical** [1173]. **diagrammatics** [1942]. **Diagrams** [846, 761, 87, 1585, 18, 1495]. **diamagnetic** [1378]. **diameter** [1250, 1298, 1239, 1063]. **Diamond** [2150, 1104, 1979, 284]. **diamondoids** [2150]. **Diastereomeric** [820]. **diatom** [3290]. **diatomic** [2034, 2032, 1556, 1514, 2879, 2614, 113, 2513, 3526, 659, 2099, 1481, 3727, 2985, 2149, 1469, 1980, 3523, 35, 732, 545]. **diatomics** [250]. **diatropicity** [1492]. **diazene** [1662]. **dicarboranes** [2037]. **dication** [2393]. **dichalcogenide** [2687]. **dichotomous** [378]. **dielectric** [1553, 2521]. **Diels** [2094]. **diesel** [2929]. **DifEquns** [3089]. **DiffEqns** [3077]. **DiffEquns** [3092]. **Difference** [3405, 3106, 2908, 2828, 3483, 2815, 2943, 3712, 1750, 3653, 1045, 3231, 3040, 2855, 3172, 3269, 2529, 1725, 3509, 2844, 3573, 2880, 3014, 3160, 3038, 2803, 2816, 2719, 3134, 2834]. **differences** [3023, 3025, 3516]. **Different** [3018, 1152, 2940, 3284, 3307, 224, 2715, 3145, 1194, 1303, 2127, 2126, 1723, 1724, 2489, 7, 3675, 3506, 1409, 1340, 3688, 3492]. **Differential** [842, 3299, 903, 2155, 189, 3235, 905, 748, 1166, 1084, 2180, 1666, 1797, 1696, 1697, 1984, 2254, 3685, 1692, 1655, 1392, 2386, 3575, 3598, 3404, 1912, 2089, 2090, 645, 3082, 2319, 2320, 2695, 2888, 3544, 656, 1950, 2556, 1842, 3440, 3725, 2795, 2718, 2507, 2271, 3412, 3435, 2232, 2546, 3197, 2389, 2475, 3391,

3693, 2428, 2328, 2135, 2302, 1644, 2745, 3208, 3134, 1816, 3212]. **differentiation** [1184, 3350, 3406]. **diffraction** [677]. **DiffrntEqutins** [3131]. **DiffrntEqutns** [3130]. **diffuse** [2850]. **Diffusion** [2278, 901, 861, 3451, 1152, 405, 775, 745, 757, 1150, 3106, 2658, 2875, 2832, 3713, 3565, 2386, 2210, 3383, 3687, 3660, 3330, 3307, 3103, 1740, 3589, 1078, 1935, 2502, 2884, 2517, 2447, 2927, 2085, 2245, 1316, 1190, 1334, 1562, 1710, 1714, 1715, 3699, 3712, 2308, 2359, 3607, 3363, 2955, 3034, 3726, 3397, 3653, 2808, 2811, 1292, 1689, 2219, 3055, 3110, 2974, 2244, 2583, 3008, 1718, 450, 719, 1215, 2718, 2796, 2488, 3074, 2119, 2284, 1386, 1781, 1519, 3101, 3595, 2405, 3509, 2470, 3667, 2921, 3405, 3467, 3584, 2116, 558, 3249, 1823, 1794, 3279, 682, 591, 2577]. **diffusion** [2929, 3690, 3208]. **Diffusion-Controlled** [757]. **diffusion-flame** [2447]. **Diffusion-influenced** [3451]. **Diffusions** [795]. **diffusive** [3298, 1714, 1715, 3571, 3454]. **Digitally** [1013]. **diglycosides** [1801]. **digraphs** [297, 1580]. **dihalides** [1694]. **Dihedral** [3339, 2366]. **dihydro** [1621, 1102]. **DIIS** [1872]. **dilatation** [141]. **dilemma** [572]. **dilute** [1807]. **dilution** [1276]. **Dimension** [772, 887, 789, 654, 2459, 2461, 2706, 2879, 1881, 2075, 3171, 117, 1986, 3706, 2721, 1399, 3444, 2900, 2305, 3505, 2460, 2462]. **Dimension-Dependent** [887, 654]. **Dimensional** [750, 815, 914, 916, 822, 1022, 766, 877, 823, 492, 1224, 1870, 1797, 2514, 3738, 918, 2453, 1815, 3481, 2832, 66, 122, 3413, 414, 470, 984, 1346, 1893, 2634, 3076, 3255, 1770, 3383, 1736, 3353, 1079, 2468, 2465, 3361, 435, 169, 2424, 217, 2642, 2715, 2820, 101, 323, 2688, 991, 1229, 2243, 1205, 1284, 1338, 1385, 1468, 1604, 587, 1007, 2026, 2359, 2297, 965, 3650, 84, 447, 2247, 3262, 1299, 2700, 1207, 3679, 1812, 3040, 3403, 1850, 26, 156, 2336, 2718, 2668, 2038, 3669, 1721, 647, 2405, 3016, 1491, 3603, 3112, 1837, 1302, 537, 1879, 1411]. **dimensional** [2239, 3211, 347, 522, 482, 560, 622, 3042, 3348, 1387, 1446, 1759, 3222, 1727, 1892]. **dimensional-scaling** [1736]. **Dimensionality** [2570, 2188, 13, 164]. **Dimensionlessness** [808]. **Dimensions** [942, 778, 789, 3182, 2362, 1665, 257, 2201, 3408, 519, 1967]. **dimer** [1197, 1198, 2617, 2467]. **dimer-dimer** [2467]. **dimers** [3094, 3204, 3709]. **Dinormal** [1833]. **diode** [719]. **diophantine** [3283, 3716, 777, 1036]. **dioxide** [2240, 1922, 2845, 2492, 3136, 1532]. **dipeptide** [1763]. **diphenolase** [1704]. **dipolar** [400]. **Dipole** [2972, 379, 1096, 2035, 3068, 2078]. **dipoles** [1721, 573]. **diprotic** [3524]. **dipyrimidine** [2750]. **Dirac** [685, 3009, 2466, 3472, 3514, 1612, 960, 1940]. **Direct** [2073, 1647, 2180, 2000, 2115]. **directed** [1555, 2752, 1404, 353]. **Direction** [3730, 1046, 71]. **directly** [1434]. **Dirichlet** [1982, 648, 3040]. **Dirichlet-like** [1982]. **DIRK** [2848]. **disappearing** [3426]. **disconnected** [1910, 1611, 1783]. **discontinuities** [385]. **discontinuous** [3106, 692]. **discovering** [3647]. **discovery** [3646, 3530, 407, 3067]. **discrepancy** [2603]. **Discrete** [914, 1034, 1244, 138, 598, 2188, 2421, 2841, 2944, 3455, 3661, 2184, 1852, 692, 3101, 2979, 2745, 1520]. **discrete-time** [2841, 2944, 3455, 2979]. **Discretization** [625, 3157, 656, 624, 3575, 1816]. **Discriminant** [761]. **Discriminating** [422]. **discrimination** [620, 3366]. **Discussion**

[927, 1052, 904, 690, 1805, 3164]. **diseases** [3642]. **disentangling** [1389]. **disequilibrium** [2001]. **disguised** [3531]. **disjoint** [2726, 3248]. **disk** [3663]. **disorder** [1803]. **disordered** [2832, 1416, 1518]. **dispersion** [1490, 408, 663, 2525, 3670]. **displacement** [452]. **displacements** [2799]. **dissimilarity** [1952, 486, 474, 1667, 1539]. **dissipation** [2518, 2893, 3189]. **Dissipative** [2195, 2428]. **dissociation** [726, 2413, 2512, 1532]. **dissociation-recombination** [2512]. **dissociative** [2913]. **dissolution** [2225]. **dissolved** [2762]. **Distance** [2934, 2945, 3200, 2965, 612, 807, 2824, 1144, 887, 368, 1467, 2663, 2825, 441, 1353, 148, 2555, 1576, 962, 3143, 394, 2310, 305, 2797, 290, 3230, 3293, 321, 2576, 679, 406, 270, 1259, 3555, 1473, 1672, 1652, 1502, 1593]. **Distance-based** [2965, 2663, 3143]. **Distance-restricted** [2824]. **distance-unbalanced** [3293]. **distance-unbalancedness** [3230]. **Distances** [2654, 827, 588, 438, 208, 1952, 2106, 423, 340, 573, 1473, 1719, 1539]. **distillation** [3427, 3675]. **distinct** [1359, 37, 3529, 1617, 1426, 1540]. **Distinctive** [2404]. **Distinguishable** [1948]. **Distorted** [1232, 2951, 3576, 99, 2992]. **distortion** [3541, 672]. **distortions** [3694, 2093]. **Distributed** [903, 769, 511, 648, 1934, 3059]. **Distribution** [909, 1348, 505, 362, 1868, 1553, 3730, 2390, 1465, 1466, 712, 2046, 970, 2630, 2175, 956]. **distributional** [2177, 2199, 2313, 2065]. **Distributions** [1070, 3124, 3207, 2131, 2860, 1770, 2003, 2421, 325, 2682, 947, 2009, 2700, 2911, 2224, 644]. **Distributive** [2640]. **dithiophene** [2420]. **divergence** [3311, 3651]. **diversity** [2555, 2677, 1774, 2323, 2528]. **diversity-oriented** [2677]. **diversity-variability** [2555]. **divided** [3023, 3516]. **dividing** [515]. **division** [3381]. **division-free** [3381]. **DNA** [2685, 2070, 1578, 1900, 2859, 2172, 2411, 2862, 969, 1846, 1092, 2543, 2882, 1143, 1219, 1141, 1336, 2750, 3654, 1716, 2102, 1259, 2200, 810, 2273, 1295, 1339, 1557]. **DO** [1204]. **Docking** [897, 3527]. **dodecahedron** [3694]. **Does** [676]. **DOI** [1483]. **Domain** [767, 611, 2947, 3034, 553, 2031]. **Domains** [856, 673, 2757, 408, 315, 590, 1913, 3552, 3510]. **Dominance** [865, 1365]. **dominant** [3224, 2748, 2749]. **dominated** [2416]. **Domination** [3250, 2446, 2870]. **Donder** [1087]. **donor** [425, 1378]. **donors** [222]. **doped** [3655, 1003]. **doping** [498]. **Doppelgänger** [2678]. **dot** [425, 2206]. **Double** [2951, 929, 1154, 885, 1065, 1428, 945, 1186, 1210, 773, 2070, 3345, 1669, 3503, 3576, 3542, 2016, 2043, 2268, 2684, 1194, 1303, 2214, 2439, 2840, 3333, 2530, 482, 560, 622, 2883]. **double-barrier** [2840]. **double-stranded** [2070]. **double-well** [2016, 2043, 2530, 482, 560, 622]. **Doubly** [929, 1646, 3043, 3672]. **Doubly-Colored** [929]. **Downward** [938, 936, 3678]. **Doxorubicin** [3090]. **Doyle** [1291]. **DQM** [3650, 3607]. **DR** [1290]. **Dragon** [3625]. **Drawing** [2068, 166]. **DRBEM** [2484, 2758]. **Drift** [1078, 2278]. **Drift-diffusion** [1078]. **drill** [2157]. **driven** [2278, 2121, 2480, 446, 2339, 1426, 2151, 3405]. **Droop** [1512]. **drop** [20, 3470]. **Drug** [3060, 3530, 1497, 2621, 3340]. **drugs** [1800, 3631, 3626, 2791, 3527, 3642]. **dry** [1531]. **dsd** [146, 351]. **DSGT2018**

[3124]. **Dual** [811, 3680, 1229, 2457, 3563, 3605, 3620, 3581, 3591, 3562, 3534, 3719, 1290, 615, 696, 697, 3671]. **dual-group** [615, 696, 697]. **dualist** [98]. **duality** [1835]. **due** [1198, 705, 1803]. **Duffing** [3109]. **Dürer** [3710]. **during** [1733, 1662, 1577]. **DWNT** [1431]. **Dyad** [353, 354]. **Dyck** [1010]. **Dymond** [1521]. **Dynamic** [2518, 1104, 1931, 926, 1584, 315, 1195, 1656, 3694, 1676, 2800, 3324, 2216, 1811, 1699, 2348, 3670, 1330, 2273]. **Dynamical** [1515, 738, 1371, 811, 906, 3656, 2354, 3597, 3168, 3432, 3535, 1961, 1962, 675, 2657, 3519, 3665, 497, 1248, 3635, 732, 463]. **Dynamics** [828, 794, 1890, 2152, 1083, 1929, 772, 2312, 1013, 1116, 2617, 3395, 748, 2422, 2705, 472, 2397, 2406, 3710, 3022, 2434, 3337, 2483, 3590, 416, 2898, 1881, 3393, 3676, 3137, 1946, 1856, 3312, 3443, 455, 1286, 2947, 310, 1057, 1047, 2910, 1425, 3539, 2897, 2306, 3244, 642, 3147, 2900, 2013, 3408, 1290, 1410, 739, 1974, 2630, 1240, 1076, 459, 1436, 1360, 2737, 2356, 2968, 3568, 3688, 3630].

E-121 [3709]. **E-137** [3709]. **each** [2253, 2410, 2322]. **Early** [1085, 3121, 1139]. **Earth** [1640, 913]. **EAS** [1540]. **EAS1** [1540]. **EC** [1957, 593]. **ECE** [700]. **Eckart** [3126, 2174, 3002, 2013]. **eclectic** [2233]. **economical** [2734, 3264, 3378, 3253, 3278, 3364, 3300, 3268, 3280, 3269, 3370, 2720, 2775]. **ecosystem** [3560]. **Edge** [849, 822, 1827, 179, 1753, 3265, 1333, 1627, 237, 1228, 2956, 2366, 2650]. **edge-center** [1827]. **Edge-Connectivity** [849, 1228]. **edge-cuts** [1333]. **edge-Hosoya** [2956]. **edge-weighted** [237]. **Edges** [1090, 3301, 119, 1918, 3326, 1571]. **Edgeworth** [1793]. **Edgeworth/Gram** [1793]. **Editor** [1368, 1484, 3097]. **Editorial** [176, 742, 779, 129, 154, 254, 282, 308, 337, 576, 829, 1391, 1, 17, 23, 42, 49, 55, 62, 69, 78, 239, 3511, 3621, 1936]. **Edmonds** [1328]. **EF** [2947, 2919]. **EF-hand** [2947, 2919]. **Effect** [901, 1052, 2376, 425, 1029, 712, 1018, 232, 244, 2832, 3331, 1395, 1040, 2496, 3514, 955, 1383, 2562, 3171, 1664, 117, 1564, 498, 2439, 249, 664, 1378, 993, 2224, 245, 2323, 2839, 2521, 2968, 733, 734, 1478, 1620]. **Effective** [1224, 943, 2364, 2620, 1241, 241, 839, 3400, 2115, 2295, 1036, 1165, 2412, 2479, 87, 3374, 3596, 1247, 3471, 2770, 3497, 3548, 2144, 2214, 2581, 3426, 3724]. **effectiveness** [2780, 2810]. **Effects** [767, 768, 2454, 2656, 2341, 665, 611, 3685, 2587, 241, 402, 553, 243, 246, 405, 436, 652, 2031, 3629, 1534, 192, 2968, 2912, 1577, 106]. **Efficacy** [3048, 2681, 3340]. **Efficiency** [1062, 3493, 2169]. **Efficient** [750, 2544, 3565, 2210, 1811, 3594, 3217, 3739, 532, 863, 3211, 3310, 1674, 1933, 1927, 3054, 3118, 2764, 3713, 2314, 3372, 3543, 3676, 2477, 296, 2927, 3215, 3025, 3464, 3477, 3593, 3440, 3363, 3369, 3640, 3159, 3480, 3714, 2770, 2694, 3055, 2583, 3008, 3608, 166, 3488, 1331, 2558, 3281, 3672, 651, 2389, 2475, 2799, 3592, 3724, 3510, 2775]. **Ehrhart** [2066]. **EHT** [2463]. **eigen** [1804, 3356]. **eigen-characteristics** [3356]. **eigen-operators** [1804]. **eigenenergies** [3566]. **Eigenfunction** [1171, 837, 2231]. **Eigenfunctions** [1081, 574, 547, 688, 3566]. **Eigensolution** [3267]. **eigensystems** [714].

Eigenvalue [87, 325, 1171, 1850, 788, 825, 557, 2154, 2016, 2043, 2751, 1576, 1748, 2872, 3616, 1282, 1382, 1940, 3209, 232, 89, 215, 1044, 1054, 1253]. **eigenvalue-based** [3209]. **Eigenvalues** [2006, 792, 2817, 2191, 821, 864, 40, 215, 1757, 1791, 3010, 328, 3616, 293, 1211, 398, 3003, 3261, 1947]. **Eigenvectors** [792, 1757, 293, 3003]. **eight** [1798, 2662, 449, 2511, 1525]. **eight-step** [1798, 1525]. **Eighth** [755, 817, 554, 800, 3081, 1084, 3116, 684, 2901, 3117, 713, 2868, 2720, 3407]. **Eighth-order** [1084, 2901, 3117, 2720]. **Einstein** [1052, 1124, 3164, 3698, 2438, 3091]. **EIS** [3132]. **EIS-4B** [3132]. **Elastic** [878, 3374, 1450, 554, 3537]. **Elasticity** [1104, 981]. **Elber** [754, 666, 731]. **Electric** [919, 1029, 1153, 2278, 3738, 2362, 971, 1769, 2035, 641, 2208, 2787, 2078]. **Electrical** [773]. **electro** [3713, 2233, 719]. **Electro-diffusion** [719]. **electrocatalysis** [2388, 1824, 2036]. **electrocatalytic** [3072, 1212]. **electrochemical** [707, 1955, 2294, 1602, 1741, 2850]. **Electrochemistry** [895, 782]. **electrode** [1995, 1320, 513, 3663, 2787]. **electrodes** [707, 2999, 1671, 3072, 1003, 2388, 2067, 1212, 1824, 2036, 448, 594, 700, 2830, 3236, 1767]. **electrodiffusive** [2347]. **electrolyte** [719]. **electrolytes** [2265, 2442, 2601]. **electromagnetic** [1680, 2453]. **Electron** [1309, 801, 15, 836, 822, 1747, 2324, 887, 2140, 846, 401, 551, 583, 2084, 758, 876, 961, 2130, 329, 1348, 37, 1669, 2951, 3132, 3442, 3441, 3576, 3685, 746, 2861, 1805, 1868, 286, 338, 283, 3273, 3437, 3472, 2688, 2826, 3424, 2187, 1681, 3411, 1262, 2789, 1889, 318, 504, 2039, 747, 2652, 2600, 624, 97, 332, 363, 2169, 1138, 852, 95, 465, 1398, 1440, 1968, 2449, 1006, 2509, 3276, 2252, 2690, 3719, 1210, 737, 1859, 1488, 1569, 1903, 2627, 601, 654, 2175, 1949, 2550, 440, 2521, 1835, 106]. **Electron-Densities** [401]. **electron-electron** [2690]. **Electron-pair** [1747, 2324, 961]. **electron-proton** [2861]. **electronegativities** [3617]. **electronegativity** [3319, 970, 3371, 1610]. **Electronic** [918, 886, 898, 2448, 1105, 919, 1518, 1734, 392, 1102, 2068, 141, 974, 216, 567, 743, 1744, 1805, 2843, 391, 2376, 3526, 971, 1447, 248, 3417, 3418, 3366, 251, 125, 96, 437, 1432, 1349, 1382, 1645, 1622, 2104, 2382, 2497, 1855, 133, 1939, 3452, 2912, 350, 1522]. **Electronic-geometric** [1734]. **electronics** [3655]. **electrons** [2180, 708, 1236, 978, 1268, 2918, 2183, 3418, 1966, 1300, 933, 956]. **electronuclear** [1971]. **electrophilicity** [3177]. **electrospinning** [3297]. **Electrostatic** [2538, 2003, 2421, 2203, 1973, 202, 620, 533, 3249]. **electrotopological** [3627, 167, 2133]. **element** [1989, 960, 2988, 389, 390]. **Elementary** [807, 1611, 1283, 1910, 2019, 336, 738, 3154, 3556, 694]. **Elements** [476, 887, 1028, 1059, 2341, 2983, 379, 1951, 485, 613, 332, 363, 3478, 1592, 1039, 473, 575, 2661, 1329, 1511, 3190, 3191, 3192, 452, 532, 654, 1947, 3128]. **eliminated** [2746, 3253, 2733, 3187]. **Elimination** [1082, 1674, 1927, 435, 1642, 3047, 111, 211, 1711]. **ellipsoidal** [2600, 1491]. **elliptic** [3361, 2346, 2850, 3276, 3167]. **Elongated** [1431, 3694]. **elongational** [1404]. **elucidation** [1423]. **eluting** [2621]. **emancipating** [2899].

Embedded [684, 252, 2632, 2662, 2143, 2334, 3026, 2213, 242, 607, 2930]. **Embedding** [251, 1580, 546, 59, 614]. **embeddings** [2542, 2784, 2629]. **Emden** [3014, 2597, 2927, 3057, 2974, 2284, 2997, 3239, 2581, 2618, 3398, 2880, 2302, 2723]. **emergence** [1795]. **Emissions** [1080]. **EMP** [1973, 2109]. **empirical** [2940, 1514, 2099]. **Empirically** [3680]. **Employing** [1194, 1303]. **Employment** [25]. **EMPR** [2258]. **Emulsion** [1032, 1682]. **Enantiomeric** [820]. **enantiomerization** [578]. **encapsulated** [1643]. **encapsulating** [2375]. **Encapsulation** [2296]. **enchanted** [2898, 2900]. **enclosure** [3385]. **Encoded** [2741, 3206, 2602, 2740, 3205, 3500, 3538, 3570, 3697]. **encodings** [555]. **end** [214, 652, 1571]. **end-on** [214]. **end-vertex** [1571]. **Ended** [892, 2536]. **endohedral** [3317]. **Endotactic** [3579]. **Endothermic** [824, 2045, 993]. **endpoint** [3392]. **energetic** [3144]. **Energies** [1164, 3540, 1496, 2421, 222, 1875, 2424, 2564, 1543, 1831, 1189, 194, 1645, 7, 3045, 2076, 1637, 976, 1063]. **Energy** [3195, 995, 1963, 468, 924, 1021, 1882, 937, 753, 1132, 1216, 1047, 1169, 355, 1135, 1145, 1752, 840, 841, 1441, 846, 3444, 3090, 876, 3395, 2239, 906, 1158, 560, 728, 2514, 918, 2669, 329, 2412, 1236, 706, 3441, 1514, 2016, 2043, 2976, 470, 520, 2383, 2843, 3323, 1393, 1869, 1868, 2751, 1729, 2003, 2304, 338, 2765, 675, 319, 425, 113, 2496, 2408, 2533, 2872, 3526, 1328, 3437, 2187, 1681, 1665, 1262, 1659, 2789, 726, 1499, 1889, 3420, 2227, 3645, 515, 2985, 723, 724, 1531, 251, 643, 1250, 1470, 992, 1308, 1237, 1826, 1983, 1110, 1574, 1836, 1873, 2941]. **energy** [3528, 3588, 3403, 852, 1773, 3547, 406, 705, 2867, 3512, 1006, 2056, 437, 1622, 3388, 3476, 1612, 1239, 3523, 533, 1501, 3473, 3669, 189, 704, 2857, 3045, 1210, 1944, 247, 3326, 418, 1903, 2627, 2992, 1977, 2092, 2703, 2840, 67, 2331, 1285, 1048, 1311, 2521, 3059, 159, 482, 350, 3470, 2743, 3317, 727, 1397, 3442]. **energy-effect** [2496]. **energy-free** [3420]. **energy-preserving** [3645, 3528, 3588]. **Energy-time** [1216]. **Enfolded** [2153, 2665, 3164]. **Enfolding** [3255]. **enfoldment** [1892]. **enfoldments** [1893, 2112]. **engineered** [2186]. **Engineering** [959, 3015, 3008, 1358]. **enhance** [3692]. **enhanced** [2833, 2423, 2707, 1739]. **Enhancement** [1062, 2255, 1314]. **ensemble** [2902, 2947, 1765, 3723]. **Ensembles** [811]. **entangled** [3123, 3360]. **entanglement** [2264, 2539, 1410]. **Entanglements** [309]. **entering** [2296]. **enterotoxin** [394]. **enthalpies** [2197]. **enthalpy** [977]. **entities** [2748, 2749]. **Entropic** [1354, 1235, 1476, 2104, 2432, 1788, 2086, 2008, 2269, 3444]. **entropies** [3338, 3484, 3686, 3700, 3737, 3736, 3475, 2678, 3515, 3550, 2350, 3414, 2671]. **Entropy** [2316, 2596, 486, 2121, 2465, 888, 3618, 982, 1629, 1898, 1899, 1982, 3481, 434, 3273, 3389, 3490, 3437, 3472, 3479, 3525, 3514, 1679, 3727, 2559, 2628, 2505, 3416, 1623, 2497, 2667, 2619, 3476, 2263, 3119, 2123, 3551, 2706]. **entropy-continuity** [2619]. **Entropy/information** [982, 1629, 1898, 1623, 2497]. **Enumerating** [2020, 2172, 2363, 2532, 991]. **Enumeration** [3094, 543, 273, 2592, 161, 297, 1154, 786, 687, 813, 3462, 2037, 2088, 2100, 2753, 2948, 75, 853, 2692, 3338, 61, 3204, 2237, 320, 1375, 110,

991, 1229, 2298, 2299, 2371, 2372, 2450, 2584, 2585, 2907, 2936, 3145, 3456, 3457, 3468, 1811, 267, 609, 667, 221, 603, 269, 2023, 274]. **Enumerations** [109, 3710, 181, 80]. **envelope** [3431, 2923]. **envelopes** [2794, 2773, 2809, 2920]. **environment** [130, 2188, 2186, 1515, 1699, 1584]. **environmental** [2307, 241, 243, 246]. **environments** [2225, 2617]. **Enzymatic** [1136, 2875, 2185, 3086, 3294, 2368, 1888, 2419, 2281, 2616]. **Enzyme** [1876, 880, 903, 698, 1011, 798, 1352, 1858, 3022, 2344, 1926, 2095, 2357, 193, 291, 1878, 1418, 2121, 2417, 2999, 2181, 3393, 3609, 2369, 3282, 1003, 1320, 3011, 2849, 1503, 1954, 2259, 1861, 2415, 2679, 1693, 2819, 1386, 1781, 2262, 3619, 1248, 3249, 1193, 1767, 2135, 3271, 1786]. **enzyme-catalyzed** [1781, 1248]. **Enzyme-Substrate** [903]. **enzymes** [1800, 3533]. **EOS** [3537]. **EPCM** [2930]. **EPDM** [1592, 1841, 2073, 2221, 2155, 2115]. **epidemiological** [3247]. **epigenetic** [3422]. **EPM** [1592]. **EPM/EPDM** [1592]. **EPR** [1052, 3164]. **Epstein** [3410, 3095, 2061, 2425]. **equal** [224, 328, 1840, 3172, 3243, 398, 1365, 3218]. **Equation** [1114, 763, 764, 817, 1729, 1078, 888, 806, 1966, 840, 841, 1174, 775, 771, 800, 863, 912, 2338, 905, 837, 1165, 867, 889, 832, 808, 788, 3639, 2180, 2034, 954, 1224, 1870, 2373, 3129, 1745, 1754, 1798, 1871, 2060, 2029, 1956, 2118, 2178, 2253, 2410, 2322, 2544, 2524, 2549, 2472, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 966, 1559, 1479, 1527, 1526, 1972, 2553, 3463, 3722, 1858, 3501, 684, 3054, 1315, 1692, 1655, 2764, 2734, 2746, 2828, 2777, 2154, 3115, 1202, 743, 984, 2534, 3575, 3598, 3660, 625, 3517, 3155, 2468, 2337, 2162, 1472, 3487, 1740]. **equation** [3589, 3676, 3122, 3324, 2923, 2110, 2283, 2893, 3674, 3313, 3443, 3082, 610, 1950, 2245, 3057, 3065, 726, 3025, 3257, 3706, 1097, 2035, 2566, 3567, 3645, 2297, 965, 3650, 3440, 3607, 1633, 1695, 1840, 1597, 3653, 3262, 624, 2633, 2143, 2334, 2941, 3026, 3109, 3679, 1381, 2159, 2896, 3227, 3151, 2047, 2733, 2238, 3088, 2349, 2407, 2554, 2336, 964, 1098, 2024, 372, 3002, 2507, 2819, 3295, 3276, 3354, 960, 2511, 2639, 2529, 1980, 2213, 1036, 3267, 967, 1099, 1799, 1519, 3016, 1678, 2486, 3509, 3603, 3112, 3189, 3408, 968, 2211, 1266, 1271, 3573, 2380, 3199, 637, 713, 1101, 1357, 1355]. **equation** [1548, 1904, 1993, 2098, 1407, 1414, 2475, 3405, 3506, 2930, 2267, 1670, 1977, 2413, 2590, 3677, 3398, 3210, 1294, 1939, 3321, 963, 3546, 1528, 1549, 2720, 2395, 3033, 2648, 2522, 2775, 2699, 2835, 3030, 3732, 1644, 1614, 2078, 2697, 2853, 2719, 2931, 1816, 1866, 2594, 89, 215, 3198]. **Equations** [842, 1123, 1013, 3355, 870, 2658, 1666, 1797, 1696, 1697, 1486, 2901, 3118, 3117, 2344, 2343, 1807, 3713, 1955, 2498, 3673, 2082, 1808, 595, 2386, 3000, 3489, 3439, 2418, 3404, 1312, 1748, 2089, 2090, 1533, 645, 3312, 2017, 2018, 2319, 2320, 2695, 2888, 3544, 656, 1471, 1751, 2146, 2248, 3215, 2242, 2482, 3420, 1247, 2401, 3594, 3725, 1194, 1303, 2014, 2541, 2725, 2184, 3159, 1884, 3682, 3110, 2974, 3008, 1861, 1718, 2903, 2645, 1618, 2795, 1693, 2718, 3459, 3559, 2488, 2507, 3244, 2271, 189, 3412, 3595, 2232, 2333, 2405, 2470, 2992, 1837, 242, 3297, 3239, 3197]. **equations** [607, 2389, 2581, 2618, 2921, 3391, 3467, 3693, 188, 3274, 3707, 1238, 3283, 3716, 3210, 210, 2007, 2880, 2328, 2135, 2236, 2302, 2582, 2723,

2577, 2774, 64, 65, 3042, 2745, 2891, 3028, 3208, 3134, 1866, 3212, 3014]. **equienergetic** [2280]. **equilibria** [3432, 528, 3228, 3433, 948, 2925, 2301, 2382, 561, 2813, 3649]. **equilibrial** [723, 724]. **Equilibrium** [1318, 1197, 1046, 1061, 1087, 2403, 1817, 1607, 2571, 2321, 12, 3294, 488, 1765, 1047, 1283, 3113, 1626, 2128, 2129, 2342, 2545, 33, 2108, 2382, 2619, 3502, 988, 989, 2459, 2460, 983]. **equipartition** [2319]. **Equipotential** [793]. **equitability** [1111]. **Equivalence** [940, 2099, 903, 2227, 1914, 804, 61, 2000, 2657, 3462, 575]. **Equivalent** [2523]. **Erdos** [2603, 3071, 3574]. **Errata** [1008]. **Erratum** [281, 460, 630, 2784, 2501, 2664, 1755, 2235, 1600, 1464, 2638, 935, 2460, 2462, 1672, 2441]. **Error** [2261, 437, 1243, 1384, 2927, 3712, 1799, 1944, 1839, 2331]. **error-in-variables** [1243]. **errors** [1277, 1204, 2331]. **especially** [1613, 2037]. **espresso** [3429]. **ESR** [87, 3475]. **essential** [3675]. **essentially** [1910, 1611, 1783]. **established** [603]. **Establishing** [1127]. **Estimate** [1144, 2927]. **estimates** [2282]. **Estimating** [438, 873, 978]. **Estimation** [1243, 2355, 1169, 2809, 3735, 2534, 1912, 2026, 1653, 3045, 3615, 3059]. **estimations** [2920, 3292, 3500]. **estimator** [1944]. **estimators** [1384]. **Estrada** [1596]. **ethane** [991]. **ethanol** [2752]. **ether** [2492, 3136]. **Ethers** [853]. **ethoxyethanol** [3184]. **Ethylene** [820, 1155]. **ETO** [1659]. **ETOs** [1014]. **Euclidean** [1892, 1893, 3255, 3453, 442, 2310]. **Euclidean-** [3453]. **Euclidian** [1952, 2106, 2112, 1698]. **Euler** [3474, 2905, 2879, 1123, 610, 3427, 3682, 127]. **Eulerian** [3252]. **evaluate** [1352, 3553]. **evaluated** [2660]. **evaluating** [2071, 3381, 3379, 532]. **Evaluation** [3582, 917, 938, 919, 1014, 1017, 1091, 1167, 1379, 1659, 1769, 2042, 2384, 128, 936, 1033, 1185, 946, 1329, 1488, 1569, 1903, 2627, 758, 908, 2016, 2043, 145, 193, 434, 980, 999, 1321, 1246, 1483, 1471, 1603, 1737, 117, 1994, 2807, 3477, 2251, 2261, 2717, 2683, 2115, 2605, 1482, 1459, 1460, 686, 1261, 8, 651, 3058, 133, 1193, 3678]. **Evanescent** [706]. **Evaporation** [775]. **even** [2760, 3462, 3328, 40, 322]. **events** [1790]. **eventually** [2093]. **every** [2305]. **Evolution** [2899, 1319, 2900, 2397, 2406, 3337, 3142, 139, 140, 1962, 2160, 2161, 2162, 2898, 3443, 2319, 2320, 2695, 2888, 3544, 3726, 2285, 542, 2234, 2429, 3112, 3663, 2806, 3705]. **evolution-operator-invariant** [542]. **evolutions** [2090, 2160]. **evolve** [1858]. **evolver** [2898, 2900]. **Evolving** [1450, 400]. **Exact** [954, 1972, 1453, 2809, 2498, 1401, 2418, 286, 3056, 3487, 3122, 1481, 3308, 879, 3227, 2554, 2713, 1980, 652, 235, 2211, 1271, 2347, 3333, 881, 1165, 1742, 1446, 1759, 2010, 2072, 2343, 3292, 2823, 1494, 3343, 2468, 3178, 3447, 3544, 1882, 2297, 676, 1407, 1414, 2033, 2338, 2413, 1209]. **Exactly** [2082, 1181, 835, 1224, 657, 689, 2840]. **examination** [56, 20]. **examined** [1226]. **example** [2207, 2305]. **exceedingly** [3548]. **exceptional** [3360]. **Excess** [2015, 781, 2940, 1531]. **excessive** [1696, 1697]. **Exchange** [655, 1665, 1773, 1490, 2951, 3542, 2042, 3087, 3547, 2030, 676, 2092, 2963]. **exchange-correlation** [3547]. **exchange-force** [1773]. **exchanger** [3007, 1733]. **excimer** [539]. **exciplex** [3096]. **excised** [80]. **excitation** [467, 367, 1543, 2224, 1711]. **excitations** [3415, 248, 1939]. **Excited**

[2016, 2043, 866, 3182, 276, 2068, 481, 2042, 3418, 1394, 3512, 249, 2429]. **Excited-state** [2016, 2043, 3418]. **Exciton** [2396]. **excluding** [1461, 1462]. **exclusion** [1452, 2610]. **exclusive** [1723, 1724]. **exclusively** [459]. **exclusively-bosonic** [459]. **exemplified** [1773, 1835]. **Exendin** [3529]. **Exendin-4** [3529]. **exhibiting** [1621]. **exist** [3532, 676]. **Existence** [884, 1312, 3147, 3375, 2249, 2557, 3687, 416, 1313, 377, 278, 274]. **exo** [2045]. **exo-** [2045]. **Exocyclobutadieneite** [2138]. **exothermic** [2744, 699, 993]. **exothermic-endothermic** [993]. **expanding** [560, 622]. **Expansion** [1179, 1167, 1603, 1737, 1134, 1033, 805, 837, 3582, 2231, 1777, 414, 1805, 3232, 2748, 1205, 1284, 1994, 2600, 2117, 1185, 1599, 1600, 2261, 2554, 3198, 1944, 1863, 2799, 2749, 2563]. **Expansions** [876, 2417, 14, 3240, 94, 533]. **Expectation** [891, 2397, 2406, 2160, 2162, 3727, 2062, 2680, 1538, 1960]. **Expected** [2825]. **expeditiously** [510]. **expeditiously-folded** [510]. **experiment** [3384, 351, 2488, 20]. **Experimental** [158, 3582, 3004, 2069, 2193, 1717, 2874, 3001, 2157, 2929]. **experimentation** [662]. **experiments** [2216, 507, 3434]. **expert** [165]. **experts** [128]. **explaining** [3119]. **Explicit** [2180, 763, 764, 2842, 2852, 2392, 2544, 2524, 2549, 2472, 2632, 2662, 1777, 2110, 2319, 2320, 2695, 2888, 1695, 1597, 2652, 2143, 2847, 3055, 1540, 713, 2098, 2317, 2381, 2370, 2455, 3102, 2868]. **Exploiting** [1687]. **Exploration** [1522, 723, 724, 3635]. **explorations** [169]. **exploring** [3680, 1622]. **explosion** [1628, 1908, 3153, 2471]. **exponent** [3233, 1220, 2267]. **Exponential** [755, 1114, 3449, 1132, 879, 860, 1033, 1678, 832, 1278, 1858, 1815, 3247, 3636, 3676, 1891, 2684, 999, 1321, 1338, 1603, 1737, 3610, 1133, 2694, 1185, 3459, 3559, 3461, 1645, 1785, 2780, 2810, 3362, 1475]. **Exponential-** [879, 860]. **Exponentially** [1114, 817, 1122, 2848, 806, 964, 1174, 912, 2522, 2697, 1912, 3674, 1510, 1098, 637, 1101, 1993, 2868]. **Exponentially-Fitted** [817, 912, 1114, 637]. **exponentials** [2842]. **exponents** [1803, 1967]. **exposure** [1699]. **exposure-based** [1699]. **expressed** [2390]. **Expressing** [1179]. **Expression** [204, 945, 2383, 2873, 121, 1995, 419, 452, 1862, 1209]. **Expressions** [1173, 508, 2660, 1827, 2843, 2999, 608, 1591, 3011, 74, 2613, 35, 356]. **extendability** [2824]. **Extended** [3031, 743, 3277, 1118, 2293, 526, 2463, 3375, 2434, 2125, 3137, 3443, 3706, 992, 1820, 3139, 1756, 3321, 350, 349, 1560]. **Extended-Rydberg** [1118, 992, 1820]. **Extending** [520, 1878, 2789, 2430]. **Extension** [2573, 3275, 206, 2900, 1069, 1696, 1697, 3501, 348, 952, 2161, 2320, 2888, 155, 3461, 302, 596]. **extensions** [2757, 1984, 441, 511, 2129]. **extensive** [1941]. **external** [974, 2412, 691, 2741, 1943, 3547, 1538, 44, 2208, 1382, 3394]. **Externally** [2708]. **extinction** [1564, 1512, 1301]. **extract** [1612]. **Extracting** [1118, 1388]. **extraction** [2842, 2748, 3675, 2749]. **extracule** [133]. **Extrapolation** [1638, 2740, 1038, 1743, 376, 3310]. **Extremal** [1176, 3238, 3148, 298, 1168, 843, 1148, 711, 869, 292, 238, 399, 3341, 1222, 1230]. **Extreme** [3271, 2391]. **extreme-ultraviolet** [2391]. **Extremely**

[3496, 3504]. **extruder** [2046].

F.R.S [18]. **Faber** [3071]. **Face** [2053, 1827, 3694, 2726, 1806, 461]. **face-center** [1827]. **Face-spiral** [2053]. **faces** [1268, 1416, 2918]. **facet** [3201]. **Facilities** [755]. **Factor** [791, 3468, 1256, 175, 3434, 3733, 350, 349, 1000, 3457]. **Factor-group** [3468, 3457]. **factorisation** [10]. **Factorization** [139, 140, 170, 83, 3062, 2554, 1988]. **Factors** [71, 304, 608, 2973, 3078, 2652, 2265, 2442, 2601]. **Failure** [1868]. **FAIMS** [1928]. **Families** [3173, 790, 3023, 2456, 3516, 2778, 3084, 1847, 2501]. **Family** [755, 2595, 1114, 3439, 782, 3569, 863, 832, 2130, 1798, 1871, 2392, 2632, 2673, 1559, 1479, 3053, 3118, 3602, 2478, 2483, 2760, 2761, 645, 2642, 1950, 2312, 2566, 3107, 2645, 1099, 1540, 968, 637, 1355]. **Fan** [3126, 2099, 2145]. **Fang** [1297]. **Fangzhu** [3181]. **far** [33]. **far-side** [2769]. **Fast** [1085, 756, 1107, 3676, 3701, 980, 874, 3702, 708, 3224, 1453, 1454, 1669, 1668, 2608, 2579, 2602, 2794, 2702, 2809, 2967, 3083, 3320, 3358, 3538, 3542, 3604, 3570, 3720, 3697, 462, 2435, 1472, 1707, 2447, 1836, 2974, 1764, 3327]. **fast-converging** [2974]. **fast-time** [2447]. **faster** [3492]. **FD** [3077, 3186, 3073, 3063, 3218]. **Fe** [2376, 3641, 632, 498]. **Fe-doping** [498]. **Feasibility** [3083, 3246]. **Feature** [1520]. **Features** [1163, 3123, 287, 2048, 2049, 947, 182, 1704, 2900, 2630, 2212]. **featuring** [1765]. **feedback** [2658, 2517, 1552, 3502, 2616, 1857, 3348, 1658]. **feedbackward** [1789]. **feedforward** [1789]. **FEM** [1928]. **fence** [299]. **Fenton** [2631]. **Fermat** [2731, 2782, 3275, 2650]. **fermentation** [120, 1656]. **Fermi** [338, 3472, 3514, 655, 551, 189]. **fermion** [3190, 3191, 3192, 1612]. **Fermionic** [108, 3360, 3421, 2469, 2212, 3498]. **ferrite** [3612]. **ferroin** [450, 477, 495]. **ferromagnets** [2655]. **Feshbach** [1971]. **Feshbach-like** [1971]. **Feus** [3466]. **few** [2712, 2826, 3424, 2173]. **few-electron** [2826, 3424]. **few-particle** [2712]. **fewer** [2025]. **Feynman** [728, 37, 2394, 18]. **fiber** [3387]. **fibers** [706]. **Fibonacci** [24, 50, 3633, 509, 3584]. **fibres** [2786]. **fibroadenoma** [2431]. **Field** [3206, 1105, 919, 1116, 809, 840, 841, 1029, 401, 1161, 1062, 2278, 3738, 974, 2412, 1508, 3205, 951, 374, 1948, 500, 476, 2362, 2742, 971, 1769, 1001, 228, 2426, 3547, 1538, 641, 1041, 2208, 635, 1043, 312, 2348, 2561, 663, 1532, 2239, 389, 390, 3671]. **Field-Based** [809, 1041]. **field-flow** [663]. **field-theoretic** [1508]. **Fields** [1030, 1066, 831, 819, 2453, 691, 1049, 1286, 1705, 1639, 44, 3357, 533, 3394, 277, 1314]. **Fifth** [889, 2549, 3107, 3510]. **fill** [2353]. **filling** [2969, 214]. **film** [3713, 2085, 3065, 3016]. **film-pore** [2085]. **films** [2694]. **Filter** [1081, 1459, 1460, 2635, 3158, 3348]. **filtering** [2808]. **filtration** [2624, 3020]. **filtration-absorption** [3020]. **find** [2468, 1426]. **FinDiff** [3089, 3217, 3243]. **Finding** [3185, 1480, 1836, 1825, 2440, 2647, 462, 3259, 3372, 1873, 1434, 1766, 3272, 2891, 3407, 2441]. **fine** [2827]. **finer** [2339]. **fingerprinting** [1331]. **Fingerprints** [1079]. **FinitDiff** [3092]. **Finite** [759, 1081, 823, 2908, 2828, 3483, 217, 476, 2815, 2943, 2727, 3740, 3742, 1750,

410, 3231, 3040, 2306, 2855, 3172, 3269, 960, 2529, 1329, 1511, 3488, 2675, 3509, 2844, 2428, 2880, 3014, 2239, 3160, 2805, 2988, 2803, 2816, 389, 390, 2277, 2719, 3134, 2834, 1402, 1253, 1446, 1759]. **Finite-Dimensional** [823, 217, 1446, 1759]. **FiniteDiffr** [3130]. **FiniteDiffrnc** [3131]. **First** [3655, 2674, 2130, 1745, 1754, 1871, 2029, 2178, 2253, 2392, 2410, 2322, 2544, 2524, 2549, 2472, 2673, 2623, 2662, 2691, 2709, 1692, 1655, 1287, 1288, 1289, 1805, 2103, 2337, 1225, 3652, 3662, 2556, 3170, 547, 2849, 1685, 2105, 2499, 2132, 2633, 3378, 3714, 566, 1966, 2733, 3364, 2507, 2271, 1612, 2511, 652, 2889, 699, 1904, 2317, 2381, 2455, 2930, 3370, 3707, 1500, 1845, 1222, 3556, 1264, 3211, 2302, 2648, 3030, 2594]. **first-** [547]. **First-order** [2674, 2130, 1692, 1655, 1225, 2105, 3714, 1966, 1612, 652, 699]. **First-principle** [3655]. **first-rate** [3662]. **Fisher** [3009, 3559, 2486]. **fit** [2304]. **Fitted** [817, 806, 1174, 771, 863, 912, 1956, 966, 1114, 3130, 1912, 2848, 3674, 3089, 3012, 3109, 3141, 3152, 3739, 964, 1098, 2024, 967, 1099, 3569, 2380, 637, 713, 1101, 1357, 1355, 1993, 2868, 3081, 2331, 1549, 3033, 2522, 2697, 2698, 2853]. **Fitting** [755, 3400, 3395, 832, 3493, 3735, 3504, 3662, 3596, 1194, 1303, 3378, 3480, 3471, 3692, 3364, 3300, 3497, 3548, 3586, 3608, 1717, 3046, 2201, 3675, 1678, 3370, 3426, 3689, 1756, 3592, 3724]. **fittingness** [2584, 2585]. **Fitzhugh** [2248]. **five** [3132, 2856, 1618, 2844, 3187, 2876]. **five-stages** [2856, 2844, 2876]. **fixed** [2478, 2298, 2371, 2588, 2084]. **fixed-point** [2298, 2371]. **Fixing** [1016]. **Flag** [1964]. **Flame** [812, 824, 2447, 2454, 3074]. **flames** [3330, 2562, 2119, 993]. **Flammability** [894]. **Flat** [861, 2134, 1409]. **flavylium** [1641, 1976]. **flax** [2786]. **flexibility** [705, 164]. **flexible** [100, 3139, 730]. **flight** [2488]. **flip** [2396]. **Floating** [3717, 3319, 3499]. **flounders** [75]. **Flow** [997, 1020, 828, 861, 1849, 1880, 2802, 2152, 2114, 2247, 2480, 2551, 2046, 3669, 2758, 663, 3102, 2525, 3571, 2774, 2051, 2354]. **flowcharts** [3138]. **flows** [2339]. **fluctuating** [3050, 2779]. **Fluctuation** [1810, 2406, 2121, 1582, 1778, 1779, 2470]. **fluctuation-limited** [2470]. **Fluctuationlessness** [1666, 1777]. **fluid** [2082, 3408, 2758, 3571]. **fluidized** [1780]. **fluids** [2495]. **fluoranthenoid** [1701]. **fluoranthenoid/fluorenoid** [1701]. **fluorenoid** [1701]. **fluorescence** [2337]. **fluoride** [2917]. **fluorite** [1932]. **fluorspar** [1932, 1691, 1925]. **Flux** [801, 2403, 1710, 3488]. **flux-corrected** [3488]. **flux-force** [2403]. **fluxes** [1767]. **FN** [2248, 2248]. **Fn.** [615]. **foam** [3255]. **Fock** [1366, 1471, 1595, 1455, 386, 722, 3155, 796, 1151, 3420, 2169, 2184, 333, 449, 3382, 2205, 2113, 572]. **Fock-like** [3382]. **focused** [2677]. **Fokker** [3262, 624, 2405]. **folarrs** [2089]. **fold** [342, 1290]. **folded** [2089, 510]. **folding** [499, 291, 453, 510, 3529, 2477, 2947, 1619, 2031, 1913, 653, 136]. **folding/unfolding** [653]. **folds** [1847, 2599]. **followed** [3556]. **Following** [1142, 754, 666, 1711]. **food** [2517, 1356, 1310, 1373, 1276, 1823, 1254, 1317, 1231]. **food-limited** [2517]. **Force** [831, 819, 2403, 374, 1412, 2019, 1705, 1639, 1773, 1464, 1463, 378, 1404, 2799, 2023]. **force-induced** [1412]. **Forced** [556].

Forced-convergence [556]. **forces** [1490, 2802]. **Forcing** [1125, 2958, 147, 3270, 3336, 2569, 1263, 1178, 1249]. **Foreword** [2886, 742, 779, 129, 282, 3097, 176, 154, 254, 308, 337, 576, 1, 17, 23, 42, 49, 55, 62, 69, 78, 239]. **forgotten** [2500]. **Form** [547, 887, 2180, 330, 397, 2866, 1037, 1103, 1283, 2852, 2567, 28, 485, 1521, 99, 2073, 2221, 2295, 2489, 2711, 2207, 3459, 444, 2256, 601, 3715, 671]. **Formal** [1667]. **Formalism** [1020, 796, 566, 1655, 2862, 1887, 1888, 1278]. **formalisms** [564, 245]. **formamide** [3184]. **format** [3000, 3443]. **formate** [3330, 3074]. **Formation** [2575, 1405, 2875, 1971, 2412, 1457, 1458, 977, 2724, 3103, 1685, 2980, 2869, 3617, 1561, 2262, 2978, 3272, 2197, 3454, 3690]. **formed** [1359]. **forming** [3438]. **Forms** [1015, 748, 1979, 2415, 322, 3283, 3716, 2302, 522]. **Formula** [1046, 2966, 638, 617, 2150, 25, 1640, 3664, 80, 1701, 3294, 3301, 2564, 2684, 132, 1051, 2789, 3149, 1752, 3512, 1337, 127, 3406, 2926, 3038]. **Formulae** [786, 1167, 456, 1603, 1737, 1996, 1599, 473, 1357, 1993, 3362, 1600]. **formulaes** [1334]. **Formulas** [896, 2390, 575, 1988, 1438]. **Formulation** [862, 139, 3334, 276, 2373, 416, 1961, 2748, 3135, 3420, 1909, 343, 402, 2047, 548, 507, 3210]. **Formulations** [1073, 1087]. **forward** [2684, 3047]. **forward-peaked** [2684]. **found** [2207]. **foundation** [1952, 471, 1961, 1962, 488, 280, 666]. **Foundations** [942, 1173, 647]. **Four** [1578, 2180, 2118, 2178, 2253, 2410, 2322, 2544, 2549, 2472, 2938, 3039, 3542, 2820, 2688, 1205, 1284, 1338, 1385, 1468, 1604, 3012, 342, 2798, 2633, 1207, 2847, 3450, 573, 1101, 1355, 2098, 2317, 2370, 2455, 2648, 2994, 3028, 3271, 1569]. **four-body** [3542]. **Four-component** [1578, 1604]. **four-dimensional** [1205, 1338, 1385, 1468, 1604, 1207]. **four-electron** [2688, 1569]. **four-stage** [3271]. **four-stages** [2938, 3039, 3012]. **four-step** [2118, 2178, 2253, 2410, 2322, 2544, 2549, 2472, 2847, 1101, 1355, 2098, 2317, 2370, 2455]. **four-valent** [342]. **Fourier** [1483, 3538, 3604, 3570, 3720, 3697, 836, 427, 1081, 2117, 3109, 2716, 1482, 1160, 3042, 1520]. **fourteenth** [3493, 3504, 3662, 3596, 3692, 3497, 3548, 3586, 3608, 3689, 3592, 3724, 2719]. **fourteenth-order** [3493, 3504, 3662, 3596, 3692, 3497, 3548, 3586, 3608, 3689, 3592, 3724]. **Fourth** [3645, 2544, 2524, 2549, 2623, 2662, 3660, 3439, 2483, 2892, 527, 3107, 2733, 3459, 3508, 3559, 2507, 2511, 3603, 2335, 3391, 3705, 2428, 646, 2594]. **fourth-** [2892]. **Fourth-order** [3645, 3660, 3439, 2483, 527, 3603, 2335, 3391, 3705, 646]. **Fowler** [3239, 2618, 2723]. **Fox** [2952]. **FPDP** [1639]. **Fractal** [3324, 757, 3171, 117, 745, 2599, 164, 1967, 3208, 3222]. **Fractional** [2811, 3639, 3054, 3673, 2386, 3575, 3598, 3660, 2418, 3404, 3517, 2282, 3676, 2517, 2146, 2248, 3215, 3025, 3668, 3567, 3369, 3616, 3653, 2808, 3679, 3682, 3633, 2415, 2679, 2488, 2989, 3412, 2232, 2405, 3509, 3603, 3552, 3359, 3405, 3584, 2822, 3705, 3677, 3546, 3208]. **fractional-order** [2822]. **fractionally** [2448]. **fractionation** [663]. **fractions** [2344, 1451, 1591]. **Fragment** [1969, 1970, 1968, 3214, 2655]. **fragmentation** [3488, 440]. **fragments**

[25, 243, 45, 982, 1790, 2382, 3622]. **Frame**
[916, 2169, 2174, 2661, 2013, 2257]. **Frames** [886, 778]. **Framework**
[1052, 3286, 244, 3255, 499, 1987, 1283, 3340, 173, 3704, 2236]. **frameworks**
[3338, 2871, 3484, 3686, 1890, 173]. **Franck** [608, 659, 3078]. **Frank**
[3337, 71, 407, 2409]. **fraught** [3039, 3044]. **Fréchet** [1719]. **Fréchet-type**
[1719]. **Fredholm** [3355, 2407]. **Free** [846, 2229, 106, 3023, 2647, 2995, 3117,
3489, 1040, 319, 3701, 1444, 2027, 3420, 3381, 515, 2778, 1778, 2903, 705, 2385,
2305, 2857, 1810, 1285, 159, 3069, 3470, 2891, 3407, 729]. **Free-Electron**
[846, 106]. **free-radical** [1040]. **freedom** [1948, 2578]. **freely** [2562]. **freeon**
[95]. **frequencies** [59, 3045]. **Frequency**
[2350, 1256, 249, 3733, 1794, 2331, 1549]. **Frequently** [801, 1948]. **friction**
[2509]. **Fries** [2063, 2217]. **front** [3699, 495, 2151]. **Frontal** [1643, 1040].
Fronts [1029, 641, 1405, 591]. **frozen** [3516, 3418]. **FSAL** [3026]. **FSGO**
[3371]. **FT** [1707]. **fuel** [3368, 3367, 2929]. **Fues** [2552, 3512, 3566]. **Fujita**
[1154, 1229]. **Fukui** [884, 883, 949, 957, 1523, 1632, 1735, 1809, 1860, 865,
2136, 2457, 3620, 3581, 3591, 3534]. **Full**
[756, 1130, 2978, 3134, 521, 3006, 3258, 3348]. **full-dimensional** [3348].
Fullerene [803, 849, 1122, 1510, 846, 787, 1117, 3201, 627, 1257, 3179, 1554,
3614, 2824, 2414, 1333, 1627, 1474, 1228, 2607, 2932, 1565, 1746, 1732, 3248].
fullerene-based [1746]. **Fullerenes**
[1072, 2771, 2593, 2266, 1422, 1326, 1480, 3180, 2728, 2537, 2726, 1429, 1427,
2681, 1996, 365, 1650, 631, 2147, 3419, 1442, 1919]. **Fulleroids**
[760, 1115, 1437]. **fully** [3055, 3069]. **Function**
[1020, 1026, 1179, 2125, 895, 1091, 782, 860, 1118, 2306, 2837, 3709, 179, 505,
2644, 2344, 2343, 2952, 1692, 362, 479, 2016, 2043, 3207, 3664, 1287, 1288,
1289, 1351, 1792, 1805, 1953, 2196, 2103, 2136, 2176, 2383, 952, 3233, 1582, 12,
3526, 2684, 1379, 1468, 538, 3643, 2576, 2652, 992, 1237, 1521, 1826, 1983,
1465, 1466, 1599, 1600, 2261, 3581, 3534, 2683, 243, 3314, 2094, 2056, 1511,
2404, 8, 2256, 621, 136, 2335, 2400, 1500, 1845, 2204, 1810, 2050, 2459, 2461,
2460, 2462, 2706, 3144, 3211, 1829]. **Functional**
[884, 883, 1013, 333, 449, 773, 1089, 2316, 2202, 1869, 1868, 338, 2165, 1184,
2187, 1096, 648, 2556, 2567, 355, 276, 3547, 1968, 3654, 2867, 3416, 1535, 1859,
285, 646, 729, 1340, 1301, 2610]. **functionalized** [2167, 2510, 1442].
Functionals [769, 1982, 1681, 511]. **Functions**
[1113, 865, 927, 924, 917, 938, 1017, 1065, 879, 844, 860, 923, 932, 1015, 1135,
1145, 936, 758, 2526, 2586, 974, 1971, 618, 1348, 1815, 3481, 1777, 2741, 2905,
990, 996, 746, 2203, 1392, 598, 1369, 1289, 1744, 1885, 2103, 2136, 456, 1868,
213, 3296, 2519, 3145, 2216, 3017, 656, 980, 999, 1205, 1284, 1385, 1471, 1604,
1814, 3678, 2384, 632, 1747, 3726, 3262, 2039, 2105, 1909, 2390, 1308, 1325,
1469, 1820, 1350, 1456, 1764, 2261, 1613, 2457, 3620, 3591, 3421, 344, 2605,
3203, 2850, 3276, 2179, 2690, 1329, 2469, 3430, 1855, 1459, 1460, 199].
functions [365, 651, 2780, 2810, 3552, 3362, 506, 1739, 1879, 133, 961, 3211,
368, 1907, 560, 622, 1542, 356]. **Fundamental**
[1809, 801, 1523, 2534, 2716, 3177]. **Further** [323, 1136, 2093, 729].

furylethylene [1430]. **Fused** [885, 31]. **Fusene** [3585]. **Fusenes** [1199]. **Fusheng** [1297]. **future** [148, 3052, 3642]. **Fuzzy** [568, 3142, 421, 1828, 1119, 1155, 1293, 1661, 3017, 2081, 440, 1998, 3628, 1251, 1330, 1694, 2288]. **fuzzy-subset** [1694].

G [2785, 423, 1485, 590]. **G-invariant** [423]. **G-protein** [590]. **GA** [2115, 222, 425]. **GaAs** [222, 425]. **GaAs/Ga** [222, 425]. **Gabor** [648]. **Gaddum** [3143, 1854]. **Gaddum-type** [1854]. **gain** [3043]. **Gamma** [938, 3678]. **gap** [2420, 304, 1543, 3326, 3145]. **gapped** [3009]. **Garnet** [1152, 3307]. **Gas** [856, 822, 673, 2976, 1931, 2210, 1395, 1681, 674, 1618, 2788, 712, 2263, 3119, 250, 1766, 1711, 1402, 1620]. **gas-liquid** [1931, 2210]. **gas-phase** [1711]. **gaseous** [2772, 2128, 2129, 2342, 2545]. **gases** [3501, 3698, 1994, 364, 3730, 988, 1061, 2806, 3058, 1977]. **gastric** [3460]. **gate** [3036, 3348]. **gating** [2391, 3671]. **Gaudin** [3202]. **Gauging** [2690]. **Gauss** [3161, 943, 1894, 1642, 3211]. **Gauss-Core** [943]. **Gaussian** [3499, 1892, 1865, 2016, 2043, 145, 1451, 1744, 1893, 2112, 3164, 3324, 3350, 2384, 3319, 1065, 3377, 3403, 2439, 3717, 133, 2582]. **Gaussian-type** [145]. **gaussoids** [2688]. **Gd** [87]. **Ge** [1544, 1543]. **gecko** [3222]. **gecko-like** [3222]. **Gegenbauer** [836, 3297]. **Gegenbauer-wavelet** [3297]. **gel** [1897, 1040]. **Gel'fand** [3339, 3679]. **geminal** [3520, 3202]. **Geminals** [1940, 541, 1941]. **geminate** [3536]. **gene** [3332]. **General** [3129, 866, 928, 3536, 457, 1121, 1996, 1909, 809, 902, 647, 3272, 1949, 2550, 1165, 1089, 3285, 330, 2887, 2995, 3117, 1443, 1655, 1865, 3183, 1287, 1952, 1176, 1220, 1472, 1728, 2923, 1265, 1053, 1133, 2807, 182, 2611, 1820, 1723, 1724, 452, 590, 3188, 2889, 3281, 3304, 3495, 3667, 306, 3154, 717, 322, 2799, 2350, 983, 3028, 1771, 1649, 1590, 344, 2528]. **General-Model-Space** [902]. **Generalisation** [1395]. **Generalised** [2338, 788, 2622, 3162]. **Generalization** [348, 2309, 238, 399, 132, 2865, 646, 729, 1793, 3389, 1702, 51, 285, 2083]. **generalizations** [1591, 105]. **Generalized** [886, 898, 691, 851, 1179, 397, 746, 362, 3234, 888, 1146, 1171, 3149, 860, 1033, 582, 163, 358, 1046, 417, 2258, 3554, 1147, 1938, 1272, 3225, 3105, 3120, 1992, 708, 3700, 1877, 2672, 114, 1598, 1885, 1915, 2782, 1804, 3410, 2878, 1252, 3701, 3496, 227, 296, 1603, 1737, 71, 3257, 3706, 458, 1910, 2863, 1219, 3166, 1465, 1466, 2159, 2896, 1185, 2140, 2713, 74, 2668, 1785, 2079, 635, 1799, 2486, 3112, 3189, 3408, 3573, 2768, 2022, 3095, 3546, 1203, 215, 1759]. **Generated** [766, 130, 476, 1665, 1194, 1303, 2677, 3249]. **Generating** [1555, 213, 365, 3296, 3553, 296, 2863, 2105, 344, 277]. **Generation** [815, 1066, 171, 1523, 1809, 260, 179, 25, 3096, 2391, 2537, 306]. **Generator** [763, 764, 846, 142, 2778]. **generators** [2928, 361, 3190, 3191, 3192, 368]. **generic** [1505]. **Genetic** [826, 740, 1841]. **genetical** [1206]. **Genocchi** [3274]. **Genome** [1144, 1467, 2952]. **genomic** [2523]. **gentlest** [2434]. **genuine** [1389, 3697]. **Genus** [1182, 2411, 586]. **Geometric** [143, 838, 404, 3524, 542, 2274, 497, 710, 933, 3123, 3390, 2109, 2188, 499, 3636,

1609, 2049, 3260, 2756, 1586, 1965, 2890, 1349, 1734, 3027, 2791, 3162, 1630]. **Geometric-algebraic** [3524]. **geometric-arithmetic** [1609, 3260, 3027, 1630]. **Geometrical** [623, 1952, 2136, 321, 1571, 369]. **geometries** [3306, 465]. **Geometry** [1893, 141, 220, 148, 3560, 394, 1874, 2961, 515, 2910, 194, 478, 1267, 1719, 565]. **geometry-based** [1267]. **germanium** [1544]. **getting** [2899]. **Gibbs** [2460, 2462, 1087, 2230, 2459, 2461, 2706]. **Gilbert** [1006]. **Gilmore** [2552]. **Girth** [1168]. **given** [2557, 1313, 1631, 297, 1192, 1250, 1575, 1090, 2650, 2821]. **glass** [1530, 309]. **glassy** [1671]. **glioma** [2829, 3098, 3288]. **Global** [3393, 1125, 2643, 850, 610, 948, 44, 695, 1974, 1302, 1594, 64, 65, 3510, 2051, 287, 1393, 3233, 2555, 15, 726, 2094, 280, 2839, 1703]. **Global/Local** [850]. **Globally** [1105, 1786]. **gloves** [579]. **Glucose** [798, 2829, 3196, 1999]. **glycidyl** [2492, 3136]. **glycolysis** [2841, 2979]. **glycolytic** [1740, 1703]. **Gödel** [3076, 2205]. **Gödel-like** [3076]. **gold** [1817, 3654]. **Goldbach** [2634, 2670]. **Goldbeter** [2170]. **golden** [103, 209, 1145]. **Goldman** [2365]. **Gompertz** [3247]. **good** [6]. **Gordan** [3637, 97]. **Gordon** [3025, 3645, 2941, 3227, 3267, 3042]. **Gould** [3192]. **governed** [161]. **governing** [2873, 453, 304]. **Gower** [1823]. **GP** [3350]. **GPITT** [114]. **grade** [1932]. **graded** [3575]. **Gradient** [919, 385, 3590, 971, 3539]. **gradients** [600]. **gradual** [1969]. **grained** [2710, 3334]. **graining** [2075]. **grains** [1733]. **Gram** [1179, 2689, 1793, 2878]. **Grand** [2306]. **granular** [2993]. **Graovac** [2768, 2846]. **Graph** [3338, 174, 781, 1067, 124, 94, 104, 2460, 3491, 3600, 3484, 3686, 2653, 2906, 3409, 3710, 3737, 3736, 2012, 168, 3201, 396, 3183, 3104, 1351, 3071, 320, 2735, 352, 361, 3301, 6, 2243, 1388, 180, 407, 81, 1831, 162, 165, 3347, 2801, 1200, 58, 3515, 1426, 119, 45, 2752, 39, 317, 288, 642, 2532, 3027, 1300, 2246, 2263, 3119, 3003, 3263, 3326, 173, 34, 232, 210, 3554, 3630, 178, 2459]. **graph-spectra** [1351]. **Graph-theoretic** [94]. **Graph-theoretical** [124, 104, 58, 642, 2246]. **graphene** [2624, 2164, 3127, 1518, 3214, 1998, 3568, 3671, 3688]. **Graphic** [291]. **Graphical** [1900, 721, 859, 929, 46, 147, 1092, 1075, 1760, 1180, 2683, 988, 1295, 3191]. **Graphite** [822, 492, 1441, 380, 382]. **graphitic** [1646]. **Graphs** [612, 224, 803, 849, 1122, 1125, 1123, 929, 753, 1121, 1164, 855, 1143, 1157, 303, 1168, 1487, 818, 1090, 810, 1172, 1147, 1158, 899, 1177, 787, 1117, 2934, 2945, 3200, 259, 226, 294, 208, 260, 85, 3700, 3737, 3736, 179, 2542, 2784, 37, 21, 105, 1555, 3252, 952, 289, 1176, 3632, 3396, 2620, 137, 3238, 3636, 1223, 1218, 1227, 2845, 271, 262, 627, 1257, 2190, 3179, 1728, 1631, 24, 50, 1554, 629, 2209, 2629, 2053, 3614, 991, 2824, 2870, 3143, 1753, 126, 263, 152, 328, 431, 969, 46, 3229, 299, 947, 1270, 1265, 3265, 264, 340, 1894, 458, 72, 86, 155]. **graphs** [1333, 1510, 1627, 1910, 342, 10, 336, 2797, 588, 1657, 1833, 1831, 162, 1474, 2681, 278, 221, 293, 357, 1192, 1250, 1506, 3175, 1110, 1298, 1574, 2122, 2374, 1581, 2318, 43, 398, 74, 1716, 237, 1239, 1964, 301, 3473, 1228, 2446, 2613, 358, 3093, 3261, 205, 223, 1726, 1806, 353, 354, 2280, 2932, 1222, 2966,

1048, 1203, 1311, 1230, 3013, 2273, 1611, 2606, 599, 3133, 3038, 300, 976, 1000, 2821, 3248, 1783]. **Grassmannian** [602]. **gravitational** [951]. **Gray** [3552]. **green** [3628, 1692, 1392, 3192, 2335]. **grid** [3345, 2569, 2374, 1859, 3573, 1947]. **grid-based** [1947]. **grids** [2958]. **GrInvIn** [1433]. **gross** [25, 1097, 3359]. **Ground** [866, 821, 864, 2429, 616, 2068, 2669, 3418, 3308, 96, 852, 1966, 2062, 2680, 437, 1235, 2992, 2175]. **ground-** [3418]. **Ground-State** [821, 864, 616, 852, 1966, 2062, 2680, 1235, 2175]. **Group** [910, 442, 1130, 780, 820, 850, 1173, 759, 162, 1182, 3741, 1089, 52, 2309, 2906, 2986, 491, 668, 443, 2490, 297, 2491, 2450, 3456, 3457, 3468, 1741, 585, 3740, 3742, 4, 5, 22, 284, 1327, 97, 332, 363, 243, 43, 3190, 3191, 3192, 592, 2753, 2948, 1843, 469, 739, 730, 525, 615, 696, 697, 324, 2805, 2052, 552]. **Group-Theoretical** [780, 820, 1173, 162, 1327]. **Group/Subgroup** [770]. **grouping** [3434]. **groupoids** [3346]. **Groups** [859, 2526, 3339, 2309, 2696, 633, 428, 442, 443, 3296, 476, 1579, 256, 3306, 269, 43, 99, 1968, 1843, 526, 64, 65, 2277]. **Growing** [2289]. **growth** [2586, 2829, 1536, 2152, 1686, 1515, 2044, 2897, 1512, 1981, 2978, 3272, 1374]. **Gruneisen** [3613]. **Grünwald** [3025]. **GSTE** [307]. **GTI** [1252]. **GTI-space** [1252]. **guess** [1676]. **Guest** [3621, 1936, 3097]. **Guggenheim** [1213]. **guiding** [2957]. **Guo** [1978]. **Guseinov** [1600, 1350, 1456, 1599, 1459, 1460, 1907]. **Gutman** [896, 3666].

H [2785, 1736, 1978, 2872, 683, 2968, 2755, 3583, 3330, 1181, 3308, 3640, 1116, 1476, 2087, 3663, 250, 3153, 1232, 389, 390, 1544]. **H-atom** [1736]. **H5N1** [1651, 2234]. **Haar** [3361, 1751, 2529, 3430, 2057, 2333, 2405, 3266, 3611, 3704]. **Haber** [2321]. **Hadamard** [2310, 3113]. **hadron** [1668]. **Haldene** [1254, 1231]. **half** [395, 1635, 1102, 3456]. **half-integer** [395]. **half-line** [1635]. **half-metallic** [1102]. **Half-size-subgroup** [3456]. **halide** [1155]. **halides** [3523, 3659]. **Hall** [3627]. **Halley** [3118, 3111]. **halogenated** [164]. **Hamilton** [1472, 1278]. **Hamiltonian** [2669, 1546, 1280, 1796, 2848, 1791, 838, 888, 3137, 1019, 1156, 2408, 2533, 3708, 1328, 431, 3025, 241, 81, 182, 1425, 3528, 3588, 835, 891, 1940, 173, 2338, 654, 1396, 881, 911, 973, 749, 646, 2881]. **Hamiltonians** [1395, 286, 87, 476, 3174, 2174, 958, 412, 1137, 413]. **Hammerstein** [2645]. **Hammond** [3525, 494]. **Han** [2515]. **hand** [2919, 2947]. **handles** [2579]. **Handling** [634]. **Harary** [2309, 3252, 213, 212, 1572, 407, 301, 1367]. **hard** [3661]. **Hardness** [865, 3233, 3490, 3319, 1610]. **Harmonic** [532, 1062, 2180, 3415, 2101, 2751, 100, 2872, 2820, 3329, 2187, 2183, 2710, 2727, 3049, 2509, 3476, 2668, 452, 3305, 2429, 2792]. **harmonic-oscillator** [2751, 2872]. **Harmonics** [1160, 2465, 2493, 1986, 2042, 3290, 1314, 1866]. **Harmonium** [1937]. **harmony** [1761]. **Harriman** [2108]. **Hartree** [1455, 722, 3155, 796, 1151, 1366, 1471, 1595, 3420, 2169, 2184, 333, 449, 3382, 2113, 572]. **harvesting** [2458]. **Hashin** [2479]. **Hausdorff** [2397, 217, 2576]. **having** [2995, 1918]. **hazard** [1699]. **HBr** [1577]. **HC** [3042]. **HD** [758, 250].

HDMR
[1299, 766, 1909, 2390, 2716, 3040, 1810, 1821, 2050, 2022, 2563, 3042].
He-Laplace [3312, 3244]. **He-like** [2669]. **Heat**
[812, 2772, 2484, 1799, 2758, 3058]. **heating** [3122, 3669, 2487]. **Heaviside**
[2033, 2338, 2576, 1407, 1414]. **Heavy** [2926, 2341]. **Heavy-particle** [2926].
HeD [2743]. **hederagenin** [1801]. **HEDT** [1805]. **heights** [2842].
Heisenberg [481, 914, 984, 2112, 2383]. **held** [3015]. **helical** [100].
Helicenes [1169, 274]. **helium** [3132, 3503, 3576, 3542, 2042, 3150].
Hellmann [728, 2394, 18, 1344]. **help** [3403]. **Henri** [2095]. **Henry** [1856].
heptacoordinate [146, 351]. **heptadiagonal** [3464]. **heptagon** [544].
heptagonal [3710]. **heptakisoctahedral** [668]. **herbal** [3675]. **Herman**
[379]. **Hermite** [3397, 3040, 875, 1004]. **Hermitian**
[2373, 866, 1791, 1019, 1156, 3174, 1382, 2218, 2396, 1939, 646, 1278]. **Hess**
[3551]. **Hessenberg** [2807]. **Hessian** [638, 665, 2154, 488, 234]. **heteroclinic**
[377]. **heterocycles** [2450, 2451, 2452, 3456, 3457, 3468]. **heterocyclic** [259].
heterodiatoms [1096]. **heterogeneity** [3144]. **Heterogeneous**
[447, 649, 2357, 623, 2631, 1911]. **heterostructure** [2687]. **heterosystems**
[302]. **heuristic** [564]. **hex** [3624]. **hex-derived** [3624].
hexabenzocoronenes [2134]. **Hexacyanoferrate** [1170]. **Hexacyclic** [885].
hexagon [41, 2625, 267, 2664]. **hexagon-shaped** [41]. **Hexagonal**
[767, 1128, 751, 1016, 1073, 843, 1919, 611, 3345, 3250, 238, 224, 152, 298,
3270, 3336, 1363, 3618, 3221, 553, 1186, 1210, 1272, 711, 1201, 1649].
Hexagonal-Square [1128]. **Hexagonite** [1074]. **hexagons** [2387, 3614].
Hexokinase [798]. **HF** [632]. **hidden** [2773, 1213, 947]. **Hierarchical**
[2907, 2936, 374]. **hierarchies** [1348]. **Hierarchy** [1019, 1280, 1156, 2491].
High [750, 1745, 2118, 763, 764, 3292, 3441, 2734, 766, 1127, 2700, 3528, 1993,
1528, 1549, 440, 3732, 1062, 2060, 2524, 2549, 2709, 1797, 3493, 2072, 2809,
3538, 3604, 3570, 1770, 2571, 3676, 3325, 2026, 1695, 2849, 1299, 3335, 3040,
2506, 3403, 2711, 3559, 2507, 2038, 2201, 647, 3509, 3572, 2380, 3199, 1357,
2098, 525, 1879, 2300, 2648, 3042, 2775, 1314, 3442]. **high-** [525]. **high-cis**
[2711]. **high-dimensional** [1770, 3040, 3403, 647, 3042]. **High-energy**
[3441, 3442]. **High-Order**
[763, 764, 3528, 3732, 1062, 2809, 3604, 3676, 3509, 3572, 2380, 3199, 1314].
High-resolution [3292, 2072, 3570]. **High-throughput** [1127]. **Higher**
[1413, 509, 830, 2995, 2842, 722, 3483, 2042, 3430, 3101, 1561, 3677, 277].
Higher-order [509, 2995, 3483]. **highest** [3242]. **Highly**
[3155, 3480, 875, 2684, 3610, 2173, 162, 3512]. **Hilbert**
[2453, 743, 2748, 277, 2749]. **Hilfer** [3412]. **Hill**
[113, 3228, 2077, 2953, 522, 482]. **Hill-series** [2077]. **Hill-type** [3228].
Hilliard [3706]. **Hinshelwood** [2589]. **Hirschfeld** [2208]. **HIV**
[3627, 1746, 2626, 440]. **HIV-1** [3627, 1746, 440]. **HKT** [1805]. **HMO** [3331].
HOA [2033, 2338]. **Hohenberg** [1805, 2176, 3257, 650, 2083]. **holders**
[2858]. **hole** [2068, 2373, 3185, 1490, 2047, 3210, 1939]. **holes**
[1390, 3322, 551]. **Holling** [1823, 2610]. **holograms** [2058]. **Holographic**

[783, 1744, 1805, 1968]. **HOMFLY** [3328, 1712, 2171, 2268]. **HOMO** [304]. **homochirality** [2885, 3337, 2285]. **homoclinic** [2676]. **Homogeneous** [872, 2046, 1234]. **homologues** [1542]. **Homomorphism** [21]. **homopolymer** [2420]. **Homotopy** [3181, 3240, 1862, 3086, 2998, 3427, 2146, 2215, 3139, 2618, 2921, 3693, 2135]. **honeycomb** [320, 1991]. **Hookean** [852, 1966]. **Hoover** [1083]. **Hopf** [3410, 231, 2517, 1974, 3518, 3095, 433, 1625, 430, 484]. **hopping** [1946]. **Hosoya** [3713, 952, 1227, 1499, 1270, 2949, 1298, 1575, 1168, 1239, 1186, 2956, 203, 1272, 1435, 1109]. **hot** [1534]. **HP** [2477]. **HPLC** [921]. **HSP70** [2946]. **Hua** [2275, 2352]. **Hubbard** [414, 470, 95]. **Huber** [1955]. **Hückel** [2463, 470, 72, 2117, 172, 2208, 592, 1048]. **hull** [183, 692, 183]. **hulls** [692]. **Hulthén** [2021, 1171, 2730, 3444]. **human** [1418, 128]. **hunt** [82]. **Hunter** [3440]. **Hush** [2261]. **huts** [1915]. **Huxley** [3594, 2333]. **Hybrid** [763, 764, 3539, 758, 2050, 2029, 2118, 2253, 2410, 2544, 3284, 1912, 2494, 2815, 3440, 3170, 1633, 1695, 1840, 2935, 2909, 3616, 3601, 2847, 3547, 1204, 2511, 2529, 2779, 2370, 3210]. **hybridity** [2050]. **hydrate** [1536, 1532]. **hydrated** [2521]. **Hydration** [1534]. **Hydrocarbon** [1274, 88, 3557, 304, 2562, 63, 375]. **Hydrocarbons** [786, 1140, 933, 329, 978, 2150, 2237, 181, 80, 1701, 50, 1262, 206, 325, 32, 2191, 185, 626, 616, 75, 112]. **hydrodynamic** [2202]. **hydrodynamics** [2779]. **hydrogel** [719]. **Hydrogen** [1021, 1286, 2218, 3738, 1546, 479, 2510, 411, 3258, 2845, 2519, 3087, 2398, 2917, 1465, 1466, 437, 683, 2119, 1300, 2660, 3663, 3256, 1522]. **hydrogen-atom** [1465, 1466]. **hydrogenic** [505, 3648, 362, 222, 425, 2030, 1378, 3715, 3452]. **hydrolysis** [3271]. **hydrophilic** [2693]. **hydrophobicity** [341]. **hydrotalcite** [970, 1069]. **hydrotalcite-like** [970, 1069]. **hydroxides** [2883]. **hydroxyapatite** [2166]. **hydroxyflavone** [249]. **Hydroxyl** [853, 1976]. **Hylleraas** [1488, 1569, 1903, 2627, 646, 729]. **Hyper** [2871, 847, 1581, 3620, 3581, 3591, 3534]. **hyper-detour** [1581]. **hyper-softness** [3620, 3581, 3591, 3534]. **Hyper-Wiener** [2871, 1581]. **hyperangular** [617]. **Hyperbolic** [3650, 2837, 3056, 1737, 3289, 3203, 2780, 2810, 3650]. **hypercube** [3085, 2983, 3076, 3315, 2570]. **Hypercubes** [2858, 3071, 3142, 2928, 2981, 3481, 2634, 2859, 2984, 3241, 2731]. **hypercubic** [2721]. **Hypergeometric** [1017, 2286, 2652, 2639, 1233, 2350]. **hypergraphs** [3574, 3482]. **hypermultiplet** [2466]. **hyperparameters** [3403]. **hyperplane** [3085]. **hyperpolarizabilities** [2015]. **hyperspherical** [496, 2465]. **Hypersurfaces** [795, 3277, 573]. **hypertrees** [3219]. **hypertrophy** [2973]. **Hypervirial** [3210, 2373, 2047, 1939]. **Hypothesis** [1162, 2430]. **Hypothetical** [1074, 1646, 169]. **hysteresis** [2518, 1197, 1198, 2067].

i-carbon [1979]. **ICCMSE** [959]. **ice** [3618]. **Icosahedral** [760, 1072, 893, 365, 631]. **icosahedron** [284]. **ICR** [1707]. **idea** [3539]. **Ideal**

[1061, 988]. **ideality** [3622]. **idempotent** [1612]. **identical** [264, 1612, 277]. **identically** [3326]. **Identifiability** [1343, 1485, 2329, 1204]. **Identification** [1710, 1714, 1715, 3527, 2794, 1587]. **identifier** [1601]. **Identifying** [2200, 1799]. **identities** [457, 1986]. **identity** [1392, 420, 2030]. **ignition** [2454]. **II** [3124, 611, 957, 1258, 2406, 25, 3206, 3358, 502, 422, 2048, 2028, 2299, 2372, 2451, 2585, 2018, 1887, 1715, 3336, 1198, 724, 667, 54, 357, 427, 332, 446, 2129, 661, 449, 864, 2127, 1724, 841, 464, 490, 3314, 514, 894, 3191, 3220, 2100, 1569, 30, 354, 701, 697, 1823, 2442, 830, 413, 65, 390, 2610, 1044]. **II-cycle** [2585]. **II-the** [2372]. **III** [87, 767, 1632, 2074, 523, 423, 2452, 1187, 2368, 1888, 276, 363, 2342, 593, 3192, 532, 1903, 1170, 31, 2601]. **ill** [2057]. **ill-posed** [2057]. **Illustrated** [768, 182, 344]. **illustration** [2952]. **illustrations** [2962]. **image** [2144]. **images** [440]. **imaginary** [161, 2429]. **imaginary-time** [2429]. **immersed** [2186]. **Immobilization** [1127]. **immobilized** [3196, 3282, 1999, 3533, 3249]. **Impact** [2568, 2635, 233]. **implement** [638]. **Implementation** [750, 483, 1443, 2255, 564, 456, 3483, 1715, 2091, 3001, 1684, 3310, 584]. **implementations** [2749]. **implicated** [995]. **Implications** [866, 1010, 2285, 2580, 2602, 451, 51]. **implicit** [2623, 3673, 3610, 3110, 3459, 3559, 2507, 1830, 1525, 3199, 3546]. **Importance** [2048, 2049, 2579, 2831, 3377, 686, 161]. **important** [1778]. **imposed** [1290]. **impossibility** [3046]. **imprecise** [3306]. **Improper** [443]. **improve** [1691]. **Improved** [2804, 2895, 1291, 1325, 3512, 3566, 2938, 1297, 2959, 2922, 539, 2943, 3005, 2960, 221, 1954, 3264, 2856, 2941, 3682, 2763, 2851, 3268, 3302, 3316, 3269, 600, 635, 2627, 2926, 1528, 1549, 2971, 2803, 2876, 2743]. **Improvement** [1009, 3194, 3066, 3203, 211, 1131]. **improvements** [1901, 3288]. **Improving** [2651, 3689, 2072]. **Impulsive** [3082, 1658, 1552, 1564, 2822, 1195, 1248, 1240, 1371, 1594, 2195, 1656]. **impurity** [745]. **inaccurate** [1947]. **inactivation** [2355]. **InChI** [1565, 1551]. **InChI-based** [1565, 1551]. **incidence** [2737]. **incineration** [1661]. **inclined** [611]. **including** [2732, 1882, 1316, 1190, 1562, 1660, 3707]. **inclusion** [1457, 1458]. **incoherent** [2614]. **Incomplete** [938, 3678, 3379]. **Incompleteness** [688, 3076]. **incorporated** [1322]. **Incorporating** [2831]. **Incorporation** [1513]. **increased** [2893, 1597]. **increases** [3492]. **indacenoid** [1701]. **Indecomposable** [2132]. **indeg** [3175]. **independence** [3730]. **independent** [3587, 3433, 1005, 965, 1909, 3377, 2925, 1174, 1332, 2113, 1473, 1148, 711, 1054, 1446, 2700]. **Index** [765, 780, 1121, 1140, 847, 1088, 1347, 1031, 1106, 1157, 1168, 1230, 1177, 3225, 3399, 3561, 716, 741, 1970, 702, 1757, 633, 2120, 721, 19, 3252, 3183, 3390, 1615, 1952, 2443, 2503, 952, 1176, 2004, 2620, 1220, 3238, 1572, 3636, 207, 1112, 1223, 1227, 3148, 224, 2942, 1728, 1609, 2049, 2299, 2372, 1706, 2500, 3652, 3666, 180, 1517, 2756, 1499, 1270, 1265, 2949, 1596, 3265, 1281, 266, 167, 3482, 3175, 1983, 1002, 1298, 3341, 2890, 3522, 1968, 39, 3461, 3521, 3425, 302, 1239, 3027, 301, 1186, 2889, 3032, 3024, 3555, 1969, 3128, 3177,

2768, 2846, 2966, 203, 1571, 2133, 1720, 1058, 1854]. **index** [1209, 1630, 1120, 1201, 1217, 1771, 2821, 1367, 1342, 1566, 1502, 1590, 1589, 2528]. **indexes** [2094, 3194, 1364, 1731]. **Indexing** [1821, 2532]. **indicator** [1732]. **indicators** [2546]. **Indices** [929, 751, 809, 1147, 1109, 3683, 3245, 3624, 580, 2934, 2945, 3200, 2663, 2871, 2965, 3053, 208, 260, 61, 3481, 216, 1226, 3104, 3449, 520, 1885, 480, 1516, 3631, 1218, 2282, 1631, 1252, 186, 6, 109, 2584, 2585, 3143, 3475, 3578, 1659, 1769, 1146, 3260, 3626, 1005, 1591, 340, 305, 3515, 1575, 1581, 1372, 3029, 45, 1041, 1667, 3485, 1768, 982, 1235, 1716, 2613, 47, 3644, 3003, 1222, 2839, 3491, 3554, 1264, 3038, 2977, 1649, 1560, 1730]. **Indistinguishability** [1290]. **individualized** [2608]. **Induced** [3339, 3254, 3133, 2376, 2292, 1412, 364, 2247, 2262, 3452, 1857]. **induction** [3638]. **Inductive** [3549]. **inelastic** [708, 674]. **Inequalities** [3225, 3050, 3032, 1049, 3449, 3143]. **Inequality** [799, 1009, 3452, 679, 1131]. **Inequality-induced** [3452]. **inert** [1395, 1994, 2635]. **inertia** [3326]. **Inertial** [886, 405]. **inexact** [3031, 3108]. **inexpensive** [3497, 3548]. **infection** [3247, 2626]. **inference** [1557]. **Infinite** [865, 916, 1906, 825, 1982, 2453, 414, 3353, 1850, 3469, 1044, 1054, 1253]. **Infinite-Dimensional** [916, 1850]. **infinitely** [3579]. **infinity** [2380]. **inflection** [2154, 2041]. **Influence** [3022, 3307, 3007, 2019, 970, 1061, 2553, 3207, 3394, 2116, 2194, 558, 1739]. **influenced** [3451]. **influenza** [1651, 2234]. **informatics** [1701]. **Information** [411, 1681, 504, 3366, 2030, 2509, 1269, 2087, 2179, 3469, 1635, 2263, 997, 2068, 208, 1389, 3009, 3365, 3438, 3479, 3729, 1388, 340, 1812, 979, 982, 1354, 1235, 1624, 1629, 1623, 1622, 1898, 2008, 2382, 2345, 2527, 2497, 2667, 3444, 3458, 3119, 3551, 2200, 2233, 2671, 3628]. **information-entropic** [3444]. **Information-theoretic** [1681, 2509, 2087, 3469, 1635, 1812, 979, 3458]. **Information-theoretical** [2030]. **Informational** [2361, 2681, 2607]. **Infrared** [1618, 2464]. **Inherently** [3069]. **inhibition** [193, 1040, 1724, 1606, 1302, 1387]. **inhibitor** [3103, 3609, 3055]. **inhibitors** [1763, 3627, 1723, 1724, 3527, 1323, 3194, 1746]. **Inhibitory** [1067, 1200]. **inhomogeneities** [117]. **inhomogeneous** [2141, 2470, 2116, 2194, 2924]. **Initial** [1676, 814, 905, 2908, 2991, 2922, 3299, 2943, 1700, 2438, 2064, 3682, 2851, 2855, 3243, 3508, 1704, 1525, 3235, 2954, 2081, 1193, 2971, 3218, 3271, 3492]. **initial-value** [3508, 1525]. **initial/boundary** [2991, 2922, 2971]. **initiation** [495]. **initio** [1546, 286, 248, 1096, 318, 446, 1836, 243, 1844]. **Injection** [828, 1849]. **Inner** [560, 2324, 322, 622]. **innovative** [3584]. **inorganic** [3537]. **input** [3393, 1515, 1310, 1248, 1371, 1594, 1254, 1317, 1340, 1656]. **inputs** [1653]. **insight** [3655, 447, 2743]. **insights** [3734, 3694]. **insoluble** [2293]. **inspired** [3375, 1156, 3574, 1775]. **instabilities** [1818, 2980]. **instability** [2278, 2447, 333, 449, 562, 3454]. **instantaneous** [2369]. **insulator** [96]. **insulin** [350]. **Integer** [920, 919, 1167, 854, 1027, 1073, 811, 395, 971, 1471, 1603, 1737, 1659, 1769, 1843, 1500, 1845]. **Integer-Rank** [811]. **integer-valued** [1843]. **integers** [316, 3600]. **Integral**

[3355, 3502, 3683, 3285, 2553, 3463, 3722, 1815, 2397, 1655, 1955, 3664, 1256, 1291, 1297, 1277, 595, 1451, 3575, 2337, 999, 1051, 1986, 3420, 3725, 1350, 1456, 1599, 1600, 402, 1752, 2407, 70, 2428, 3715, 2854, 1644, 2745]. **Integrals** [836, 917, 920, 919, 1014, 1017, 1167, 1033, 854, 1027, 1160, 758, 1722, 2287, 2508, 145, 659, 2519, 971, 1321, 1379, 1246, 1483, 1471, 1475, 1603, 1737, 1814, 2042, 563, 318, 2652, 2600, 2169, 1185, 548, 2605, 2271, 1785, 1482, 946, 1459, 1460, 1261, 1491, 1488, 1569, 1903, 2627, 651, 2704, 3362, 2854, 356, 545]. **Integrated** [904, 2344, 3077, 2660, 2883]. **integrating** [1777]. **Integration** [842, 817, 1891, 1754, 1798, 2060, 2253, 2410, 2322, 2544, 2472, 2632, 1479, 617, 1777, 990, 338, 2566, 1840, 1778, 1779, 2633, 964, 1098, 2024, 1491, 1488, 1569, 2627, 1357, 2930, 3279, 1810, 1528, 3211]. **integrator** [3645]. **Integrators** [1174, 1956, 3528, 3588, 1993, 1549]. **integrity** [2435, 3296]. **integro** [2389, 2302, 1644]. **integro-differential** [2389, 2302, 1644]. **Intel** [483]. **intelligence** [193, 456, 128]. **Intense** [1116, 1062, 1286, 1043, 1314]. **intensian** [435]. **interacting** [2240, 467, 1996, 243, 2509, 3090, 573]. **Interaction** [2070, 917, 1096, 945, 825, 823, 1044, 1054, 1253, 2220, 1970, 3384, 400, 1948, 2820, 1050, 1659, 1769, 2019, 2127, 2126, 3368, 3367, 2690, 3290, 1561, 3249, 730, 2655]. **Interactions** [943, 1208, 240, 2180, 2705, 2364, 3472, 2939, 3091, 191, 1613, 2925, 3654, 1830, 2532, 247, 3629, 188, 2147, 729, 2300, 3630]. **interactive** [1406]. **Interatomic** [923, 932, 1015]. **Interconnection** [1425]. **Interconversion** [1047]. **Interdependence** [768]. **interdependent** [3551]. **Interelectronic** [887]. **Interface** [856, 673, 2210, 1856, 1935, 2863]. **interfaces** [1741]. **Interference** [3685, 2438, 1802, 2270]. **Interferences** [3091]. **Interferometry** [2300, 2912]. **interior** [3681]. **intermediate** [2951, 284, 1269, 2229, 3435, 725]. **intermediate-orbital** [1269]. **intermediates** [3146]. **Intermolecular** [1135, 240, 1659, 2710, 247, 188, 729]. **Internal** [1382, 941, 273, 135, 80, 279, 3326, 1969, 739, 1670]. **internally** [2708]. **International** [384, 1601, 959, 3015]. **internuclear** [726]. **interparticle** [2180, 2187]. **interpolating** [3017]. **Interpolation** [985, 2647, 2564, 3397, 1638]. **interpolations** [1645]. **interpret** [2144]. **Interpretation** [3501, 2661, 598, 2028, 124, 1465, 1466, 1717, 2711, 3491]. **Interpreted** [913]. **Interpreting** [2869, 2221, 2295]. **interrelatedness** [1469]. **intersecting** [2765]. **intersection** [2539]. **intersections** [1450]. **interval** [2983, 2982, 2748, 3446, 2749]. **intervals** [2675]. **intervention** [3644]. **intra** [2710, 1719]. **intra-** [2710]. **intra-molecular** [1719]. **intracellular** [1307]. **intracule** [133]. **intramolecular** [1970, 126, 683, 2532]. **Intraspecific** [3609]. **Intrinsic** [815, 629, 2209, 3443, 2961]. **Introduction** [2607]. **Invariance** [515, 1280, 279]. **Invariant** [811, 423, 3640, 3357, 542, 2474, 2257, 556, 1290, 696, 697, 2774, 1295]. **Invariants** [1138, 208, 260, 168, 352, 6, 305, 45, 317, 1619, 2791, 218, 381]. **Inverse** [3431, 3461, 2977, 3561, 996, 2976, 3652, 2187, 2852, 3175, 3522, 406, 3521, 3425, 2676, 2057, 3032, 1848, 3059]. **inverse-distance** [406]. **inverses** [3149]. **Inversion** [890, 990, 2337, 1921, 229, 1647]. **investigating**

[481, 3324, 2929]. **Investigation**
[2940, 3347, 2677, 3693, 2839, 3671, 3465, 2587, 3598, 3096, 162, 2781, 67, 1867]. **investigations** [312]. **invoking** [3068]. **involved** [1352, 1277, 451, 2512, 983]. **involving** [1955, 2800, 2383, 1602, 2337, 2355, 613, 2652, 2415, 385]. **Inward** [778, 2731]. **iodide** [1522]. **iodine** [1711]. **Ion**
[2167, 1827, 1669, 1668, 2951, 3442, 3441, 3383, 3007, 1286, 1316, 1190, 1377, 1562, 1660, 1710, 1990, 2787, 1733, 2963]. **ion-atom** [2951, 3442, 3441]. **Ionic** [943, 595, 2495, 641]. **ionicity** [2865]. **ionisation** [2093]. **Ionization** [1043, 1496, 1668]. **Ions**
[851, 2538, 2669, 2519, 2826, 1773, 2229, 2385, 189, 31, 2093]. **IPR** [2537]. **iron** [88]. **irradiated** [2254, 2344, 2905, 2952]. **irradiation** [3096]. **Irreducible** [395, 2309, 2653, 2981, 3085, 3710, 3694, 2015, 204, 476]. **Irregular** [1160, 3428, 342]. **irregularity** [3683]. **irrep** [459]. **irreps** [277]. **Irreversible** [3086, 114, 2502, 2541, 2499, 2725, 3556]. **Ising**
[1411, 1835, 1967]. **Isobaric** [1061, 988]. **isoboolean** [3375]. **Isochronicity** [2729]. **isochronous** [1808]. **Isocodal** [264]. **ISOEFF98** [665]. **isoelectronic** [2538, 995, 1365]. **Isoglitter** [2054]. **isolated** [1044, 1054]. **Isomer** [1375, 3557, 2266, 609, 667, 3462, 269]. **isomerase** [1999]. **isomeric** [1701]. **Isomerism** [868, 1579, 586]. **isomerization** [2906, 3700, 2539, 1662]. **isomerizations** [126]. **Isomers** [813, 853, 2237, 3201, 181, 2363, 1461, 1462, 603, 687, 3462, 2037, 2088, 2100, 365, 1732]. **isometric** [2540, 2547, 3634]. **isomorphic** [1539]. **isomorphism** [178]. **isoreticular** [3338]. **Isospectral** [294, 119, 38, 762, 226, 223]. **isosurfaces** [2660]. **isotherm** [1856]. **Isothermal**
[1061, 2124, 1040, 3122, 2494, 235, 988, 2921, 2963, 3615, 3102, 2881]. **isotherms** [1194, 1303]. **isotope** [665, 2272, 192, 2968, 733, 734, 1478]. **isotopic** [2706]. **isotopomeric** [525]. **isotropic** [141, 2479, 3049, 519]. **issue** [2886, 959, 3511, 3097]. **issues** [2161, 3548, 3608]. **itemized**
[2298, 2299, 2371, 2372, 2450, 2584, 2585, 3145, 3456, 3457, 3468]. **iteration** [2597, 3312, 2064, 3386, 3616, 1570, 3244, 1386, 2333, 2302, 2723]. **iterations** [2742]. **Iterative** [2701, 2515, 1238, 3023, 2995, 557, 3602, 2478, 3259, 1796, 3019, 3099, 3100, 2761, 3519, 1636, 2974, 3107, 2645, 376, 3412, 2975, 556, 3665, 3167, 3510, 2891, 3028]. **iteratively** [3432]. **Ito** [795]. **IUPAC** [171]. **IV** [2229, 1735, 105, 424, 2584, 3456, 1388, 2369, 2545, 2385, 2627]. **IVPs** [1479, 3170, 3714, 3450].

J [1483, 1455]. **Jacobi** [1451, 1472, 1278, 489]. **Jacobian** [3023, 2850]. **Jacobian-free** [3023]. **Jaeger** [2508]. **Jahn** [2653, 2906, 3694, 2093]. **János** [3511]. **jaws** [3171]. **jet** [3074, 2119]. **join** [393]. **joining** [1782]. **joint** [467]. **jointly** [3124]. **Jones**
[1877, 3577, 1760, 1883, 879, 860, 1145, 1521, 2079, 2211]. **Jordan** [2421]. **Josiah** [2230]. **Joule** [528, 2717, 3669]. **Journal** [2766, 3511, 3097]. **jubilee** [103, 209]. **July** [3015]. **jump** [2312]. **junctions** [3515, 1428, 1432]. **Junmeng** [1297]. **justification** [1736, 494]. **jute** [2786]. **JWKB** [2738].

Karplus [754, 666]. **Kaxiras** [1118]. **KB** [3205, 1801]. **KdV** [3639, 2418, 2232]. **Keizer** [2737]. **Kekulé** [3734, 41, 1417, 361, 2907, 296, 3229, 1363, 265, 153, 1429, 104, 994, 818, 75, 933, 956, 1263, 1438, 1158, 274, 1732, 2107]. **Kekulé-structure** [153]. **Kekuléan** [82, 2325, 111, 211, 274]. **kekulenes** [3475]. **Kemeny** [3301]. **Kerber** [759]. **Kernel** [1955, 2320, 2553, 3463, 3722, 2837, 1384, 2831]. **Ketones** [1106]. **key** [2255, 3730]. **Khlu** [3675]. **Kier** [3627]. **Kihara** [1705]. **Kinase** [798]. **Kind** [3355, 2337, 571, 3266, 1500, 1845, 3211, 2302]. **kinds** [2715]. **Kinetic** [1175, 1362, 1277, 1191, 1136, 3072, 674, 3420, 2686, 852, 808, 798, 997, 1628, 3284, 2189, 1352, 2185, 2311, 2343, 1926, 1202, 1256, 1762, 2383, 1869, 1868, 2751, 1878, 3258, 2812, 338, 2990, 3536, 319, 1935, 2872, 2939, 3448, 2018, 2187, 1681, 1957, 2193, 3282, 3079, 3228, 3342, 3507, 2308, 2985, 2970, 2611, 2091, 2679, 2925, 33, 1841, 2073, 2115, 2295, 2515, 2711, 2874, 3001, 2056, 2271, 1622, 1501, 444, 2675, 1903, 2627, 2779, 2978, 3272, 3707, 1616, 3351, 3649, 2574, 116, 1193, 1772, 64, 65, 2968, 3492, 2017, 1723]. **kinetic-diffusion** [1935]. **kinetic-energy** [338, 1681]. **Kinetics** [834, 903, 2499, 757, 1011, 1411, 833, 845, 1908, 2589, 2814, 1876, 975, 2518, 2732, 2644, 2254, 2905, 1655, 2357, 1291, 291, 1418, 1987, 2417, 2181, 3048, 3294, 3122, 2494, 539, 3312, 2069, 570, 2002, 3433, 3011, 948, 447, 623, 658, 2849, 2044, 1503, 1954, 2259, 1292, 1689, 344, 1693, 3728, 1985, 2207, 3244, 1504, 652, 516, 2036, 3533, 2262, 2470, 1848, 698, 3619, 1911, 1981, 3249, 2813, 3649, 2693, 3556, 2135, 2236, 3670, 3492]. **kinetics-based** [3649]. **kinky** [3585]. **KINMODEL** [1762]. **Kirchhoff** [2120, 2503, 2620, 1450, 3555, 1854, 1502]. **Klauder** [1906]. **Klein** [35, 2593, 3025, 2569, 1010, 2941, 3227, 3267, 1221, 2950]. **Klein-bottle** [1221]. **knew** [359]. **Knot** [3161, 3, 1400]. **Knots** [1108, 1894, 370, 371, 493, 312, 1304]. **knotted** [2542, 2784]. **know** [1396]. **Known** [825, 2700, 2962, 3527]. **Kohn** [1805, 2176, 2426, 3547, 650, 2083]. **Kolmogorov** [2146, 3559]. **Koshland** [2170]. **Kotel'nikov** [3120]. **KP** [3408]. **KPP** [2146, 2146]. **Kr** [1096, 250]. **Kramers** [378]. **Kratzer** [3466, 1481, 2552, 3512, 3566, 473, 548, 3425, 3267, 3394, 671]. **Kratzer-type** [1481]. **Krivchenkov** [2365]. **Kronecker** [2397, 1792, 2898, 2996, 2319]. **Kudryashov** [3150]. **Kullback** [3525]. **Kuramoto** [3706, 3559]. **Kutta** [806, 2334, 1541, 2699, 2178, 2322, 966, 1114, 1559, 2283, 2893, 3674, 2943, 3610, 1597, 2143, 3026, 3061, 2024, 2507, 607, 771, 2914, 2835]. **Kuznetsov** [3189]. **Kuznetsov-Burgers** [3189]. **Kwong** [3501].

L [752, 944]. **L-pattern** [944]. **labeled** [289]. **labeling** [2726]. **Labelings** [2593]. **Labelling** [811, 260]. **labels** [2279, 697]. **laboratory** [1937, 2069]. **laccase** [3196, 1853]. **laccase-based** [1853]. **laces** [2303]. **lactic** [1656]. **Ladder** [2468, 2620, 2365, 2275, 3566]. **ladders** [357]. **Ladenburg** [2907]. **Lag** [800, 1745, 1754, 1798, 1871, 2060, 2029, 2118, 2178, 2253, 2392, 2410, 2322, 2544, 2524, 2549, 2472, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 2908, 1559, 2734, 2746, 2893, 2566, 1840, 2778, 3084, 1597, 3264, 2633, 3242, 3471,

3253, 2733, 3172, 3186, 3243, 3278, 2507, 2511, 2380, 554, 1904, 2098, 2317, 2381, 2370, 2455, 2930, 3426, 1528, 3160, 3187, 3218, 2648, 2699, 3030, 2594]. **Lagrange** [610]. **Lagrangian** [2498]. **Laguerre** [1977, 1137]. **Laguna** [2785]. **laid** [267]. **lake** [2762]. **Lambert** [2644, 2344, 2343, 2905, 2952]. **laminar** [3074]. **Landauer** [3465]. **landscape** [2292]. **Landscapes** [807, 506, 2473, 3069]. **Lane** [3014, 2597, 2927, 3057, 2974, 2284, 2997, 2581, 3398, 2880, 2302]. **Langevin** [3383]. **Langmuir** [2589, 2553, 3463, 3722]. **Langmuir-kernel** [2553, 3463, 3722]. **lanthanide** [3655, 3418]. **Laplace** [3312, 1972, 2010, 990, 996, 3353, 2468, 121, 726, 2588, 2336, 3244, 2639, 1641, 3412]. **Laplacian** [3679, 1489]. **Large** [2315, 1089, 287, 2266, 3325, 1665, 2742, 1181, 2223, 3725, 2600, 1773, 1441, 40, 2639, 358, 2799]. **large-order** [2600]. **Large-Scale** [1089, 2315, 287, 2742]. **larger** [2053, 1806]. **largest** [1211, 232, 1264]. **Laser** [1116, 1062, 1286, 364, 2917, 1043, 389, 390, 1314]. **laser-induced** [364]. **Last** [2731, 2782, 3275]. **late** [18]. **Latent** [783, 1960]. **later** [2541, 2725, 3707]. **lateral** [310]. **Lattice** [856, 1025, 339, 346, 27, 3392, 1401, 169, 1690, 1679, 117, 2569, 267, 2228, 2177, 2199, 2313, 2559, 2628, 2615, 3140, 2505, 99, 257, 214, 3523, 672, 3188, 123, 2640, 1997, 2065, 300, 1400]. **Lattices** [793, 27, 419, 508]. **Laviron** [1671]. **law** [3587, 996, 2812, 2939, 3443, 3079, 3507, 3433, 2164, 1648, 2925, 2486, 3551, 2987, 2813, 3649]. **Laws** [3553, 2259, 2887, 990, 3115, 1049, 3020, 3257, 3706, 3151, 3016, 2031, 3667, 3112, 1772, 2487]. **Layer** [945, 2300, 773, 3070]. **layered** [629, 3368, 3367, 2957, 2883]. **LBET** [1194, 1303]. **LCAO** [1287, 1288, 1289, 1805, 1953, 2103, 2614]. **LCVW** [1065]. **Leading** [2170, 471, 2028, 378, 2285]. **leads** [33]. **leaf** [2085]. **Leapfrog** [1423, 1326, 1480, 1072, 1429, 1427]. **learning** [2039, 3340]. **Least** [2534, 872, 1770, 1533, 539, 2591, 372, 2399]. **least-squares** [1770, 1533, 539]. **Leave** [756]. **Leffler** [1026, 996]. **left** [1926, 371]. **left-right** [371]. **Legendre** [3582, 3648, 3262, 1500, 1845, 2769]. **Lego** [2722]. **Lego-like** [2722]. **Leibler** [3525]. **Lempel** [1702, 1563]. **Length** [876, 2959, 424]. **lengths** [1617, 2366, 2650]. **Lengyel** [3410, 3095, 2061, 2425]. **Lennard** [1877, 3577, 879, 860, 1145, 1521, 2079, 2211]. **Lennard-Jones** [1877, 3577, 879, 860, 1521, 2079, 2211]. **Lennard-Jones-Type** [1145]. **lesions** [2071]. **Leslie** [1823]. **less** [2962]. **Letter** [1368, 1484]. **Letters** [2]. **Level** [2305, 2253, 2410, 2322, 722, 3459, 3559]. **levels** [3195, 2829, 3431, 2408, 2533, 251, 3434, 2992, 482, 560, 350]. **Leverett** [3115]. **Levi** [2906]. **Lewis** [1383]. **lexical** [277]. **lexicographic** [702]. **Li** [2228, 2787, 1997]. **Li-ion** [2787]. **libraries** [2026, 2677]. **lid** [2480, 2339]. **lid-driven** [2480, 2339]. **Lie** [3115, 139, 140, 675, 217, 1741, 3016, 3667, 3112, 906, 64, 65, 732, 2487]. **life** [3114, 311]. **lifetime** [3124]. **ligancy** [2491]. **ligand** [476, 3036, 3629]. **ligand-protein** [3629]. **ligands** [110, 202, 1461, 1462, 2127, 2126, 2088, 2100]. **Light** [1162, 2538, 661, 250, 2458]. **Like** [767, 2669, 611, 1982, 2759, 3108, 1971, 543, 2466, 3076, 3634, 3142, 1646,

2363, 2722, 1050, 1659, 1769, 1013, 3516, 1390, 1965, 1010, 2763, 2904, 2894, 1773, 553, 3382, 642, 672, 1561, 970, 1069, 3297, 1774, 2093, 3222]. **lim** [2428]. **lim-4** [2428]. **Limit** [1225, 120, 1387, 975, 414, 470, 3287, 2748, 1665, 1181, 2159, 1773, 372, 699, 2729, 2092, 525, 2749, 1625, 987]. **limit-cycle** [3287]. **Limitations** [901, 1213, 1290]. **limited** [2292, 2517, 2409, 2470]. **limiting** [505]. **Limits** [894]. **Liñán** [1818, 2447]. **Lindemann** [3193, 3423]. **Lindstedt** [2005]. **Line** [1137, 3183, 3104, 1716, 1635, 3027, 1259]. **Linear** [777, 861, 756, 768, 2659, 2017, 2018, 2368, 2369, 32, 1834, 3355, 1065, 879, 376, 1073, 3283, 906, 1119, 2885, 2392, 2595, 2623, 2158, 1696, 1697, 1496, 707, 2330, 2485, 2644, 3022, 3086, 3224, 2254, 1607, 2237, 1692, 1655, 2777, 19, 198, 1243, 743, 931, 3004, 3315, 2503, 3226, 2812, 529, 2555, 2089, 2090, 1881, 319, 3137, 3711, 539, 1444, 1935, 2629, 1753, 736, 375, 1334, 1377, 1714, 1715, 538, 2009, 1579, 2139, 3593, 1920, 2657, 3643, 2077, 355, 2531, 1828, 3702, 1336, 3227, 2244, 1861, 1943, 3151, 1693, 2925, 1538, 3088, 33, 2221, 2141]. **linear** [3508, 2402, 2469, 1036, 533, 1519, 1100, 651, 1969, 2381, 2806, 717, 3144, 3033, 2697, 2853, 1330, 727, 1816, 734, 3716]. **linear-chain** [2469]. **Linear-Programming** [1073]. **linear-quadratic** [2254]. **linear-response** [533]. **Linearity** [330, 329, 331, 466, 884, 883, 2573]. **Linearized** [3599, 3676, 3567]. **linearly** [1395]. **lines** [2796]. **lineshapes** [2920]. **linguistic** [3628]. **link** [1490, 3294]. **linkage** [1896, 2249, 3535, 3433]. **linked** [2542, 1942, 2784]. **Linking** [2629, 721]. **links** [2444, 2004, 2268, 1274, 2020, 2172, 1524, 1709, 1894, 1760, 1883, 2543, 403, 454, 493, 3328, 1712, 2171, 1608, 349, 1755]. **Liouville** [2231, 2082, 2162, 888, 1068, 1290, 459, 3208]. **Liouvillian** [696]. **lipid** [3072]. **lipid-modified** [3072]. **Lipschitz** [3262, 3212]. **Liquid** [856, 861, 2940, 673, 595, 1931, 2210, 1618, 406, 3150, 2267, 1409]. **liquid-gas** [673]. **liquids** [950]. **list** [187, 262]. **list-processing** [187, 262]. **LM** [786]. **loaded** [3653]. **loads** [3653]. **Local** [3116, 2647, 2759, 2292, 605, 850, 3107, 2645, 3723, 3031, 260, 978, 2732, 1353, 2555, 15, 606, 6, 3437, 3257, 305, 3369, 2457, 3620, 3581, 3591, 3534, 2617, 44, 2094, 1354, 1476, 2269, 2270, 676, 2690, 3167, 3622, 961, 2839, 2331]. **local-scaling** [961]. **Localization** [2785, 1917, 1413, 1287, 190, 2097, 1803]. **Localization-delocalization** [2785, 1917, 2097]. **localized** [2986, 248, 318, 242, 2703]. **locate** [2214]. **Locating** [3345, 3432]. **locations** [1318]. **locus** [3531]. **log** [2300]. **log-normal** [2300]. **logarithm** [2661]. **logarithmic** [3110, 1810, 2582, 3732]. **logarithmic-BBM** [2582]. **logarithmic-TRLW** [2582]. **logarithms** [2952, 3283, 3716]. **Logical** [1792, 790, 456]. **logistic** [3247, 2576]. **London** [70]. **Long** [2114, 1079, 3303, 1554, 772, 1474, 922, 406, 2616, 2832, 191, 1325, 573, 2116, 192, 2300]. **Long-dimensional** [1079]. **Long-range** [406, 2832, 191, 2116, 192]. **Long-term** [3303]. **Long-Time** [772, 2616]. **Longest** [458]. **look** [2463, 2055, 650]. **Looking** [3052]. **loops** [3473, 1789]. **lore** [2111]. **Lorentz** [443]. **Lorenz** [2312]. **Loss** [812]. **Lotka** [645, 640, 115, 1276]. **Lovász** [3071]. **Low** [3206, 815, 766, 3714, 945, 845, 2544, 3205, 3538, 207, 6, 2786, 3480,

3403, 3586, 3739, 2511, 249, 3045, 1794, 67, 2422, 89, 215, 733, 1478]. **low-cost** [2786, 3480, 3586]. **Low-Dimensional** [815]. **low-energy** [67]. **low-frequency** [1794]. **Low-order** [3714, 3403, 3739]. **low-rank** [89, 215]. **Löwdin** [1142, 1350, 1456, 1599, 1600, 1764, 2400]. **Löwdin-alpha** [1764]. **Lower** [1025, 804, 821, 864, 900, 2062, 2680, 787, 3083, 408, 2959, 500, 627, 1910, 1282, 1850, 1959, 2222, 3080, 3029]. **lower-order** [3083]. **Lowest** [5, 3604]. **LQS** [2094]. **LRM** [1759]. **LS** [2229]. **Lu** [1106]. **luminescence** [990, 2504]. **luminescent** [3182]. **LUMO** [304]. **LVA** [230]. **LZ** [1219].

M [1685]. **machine** [2039, 3340]. **MacLaurin** [2879, 923]. **Macrokinetics** [364, 2923]. **Macromolecular** [465, 287]. **macromolecule** [2565]. **macroscopic** [2019]. **mad** [3350]. **mad-GP** [3350]. **made** [3646]. **Madelung** [1827, 2082, 2721]. **MADM** [2997]. **Magic** [703, 1992]. **magnet** [1102]. **Magnetic** [3721, 1085, 2072, 3206, 1153, 1139, 1389, 1453, 1443, 1901, 2255, 2431, 2608, 2651, 2580, 2602, 2741, 2794, 2773, 2702, 3066, 2967, 3205, 3320, 3358, 2426, 2750, 3547, 70, 2239, 3671]. **magnetogasdynamic** [2498]. **magnets** [1835]. **Magnus** [1863]. **Mahony** [3673]. **maintenance** [2051]. **majorization** [2120]. **making** [2656, 3628]. **malignant** [3320, 3358, 3431]. **Mandalas** [1173]. **Mandel** [1337]. **Manifestations** [1452]. **manifold** [1498, 3640, 2459, 2461, 2460, 2462, 2706, 2774]. **Manifolds** [815, 3432, 3113, 13, 2474, 556]. **manner** [1899]. **Manning** [1882]. **Many** [549, 756, 1122, 1623, 1348, 37, 2751, 1326, 2872, 2223, 1510, 2913, 3579, 2039, 97, 332, 363, 1613, 3190, 3191, 3192, 2532, 418, 1859, 1835]. **many-body** [1613, 2532, 418]. **many-electron** [37, 2039, 97, 332, 363, 1859]. **many-fermion** [3190, 3191, 3192]. **Many-orbital** [1623]. **Many-Out** [756]. **Many-particle** [549, 2913]. **map** [2447]. **mapping** [1279, 277]. **Mappings** [811, 1290, 696]. **maps** [1933, 1927, 2158, 747, 1426, 2080, 1864, 2279]. **March** [1869]. **Marching** [1107, 1472, 1836]. **Marcus** [2261]. **marginal** [355]. **Markov** [2636, 1780, 2306, 2046, 1561]. **Markov-like** [1561]. **Markovian** [2913, 1410]. **Marks** [269]. **Martin** [2165]. **Mass** [777, 834, 2009, 448, 594, 700, 1087, 1165, 1224, 2747, 2249, 2861, 3000, 1247, 3309, 1215, 1985]. **mass-action** [3000, 3309]. **masses** [1181]. **massive** [2510]. **massively** [255]. **master** [3443, 2014, 1977, 2413]. **match** [2200]. **Matching** [810, 1172, 3734, 952, 1631, 2824, 147, 170, 299, 419, 508]. **Matchings** [1025, 1122, 787, 1199, 320, 627, 1326, 1480, 152, 1510, 1192, 1211, 74, 2640, 2606, 2783, 1058, 1489, 1148, 711, 2958]. **material** [2479, 1214, 3138]. **materials** [2993, 1508, 2832, 3009, 981, 3374, 3350, 2787]. **Math** [1483, 1455]. **Mathematical** [1683, 3686, 1795, 1817, 1085, 1245, 861, 1655, 794, 927, 1287, 1288, 1289, 1805, 2103, 2510, 3103, 227, 488, 2308, 2067, 1127, 831, 819, 844, 1135, 2631, 102, 79, 1693, 2946, 3728, 795, 1999, 1588, 2962, 1512, 2766, 1691, 1170, 3663, 280, 3511, 785, 1794, 2830, 1673, 2156, 2476, 3015, 3097, 1364, 769, 484, 3635, 2912, 868, 2829, 2185, 2406, 1763, 3621, 1139, 1443, 2651, 3465, 2762, 220, 581, 273, 2225, 531, 1961, 3731, 1937, 12, 3294, 1888, 2245, 1579, 56, 256, 2972, 53, 54,

2247, 603, 3060, 314, 2128, 2129, 2342, 2545, 313, 2244, 2583]. **mathematical** [1861, 2250, 68, 77, 2332, 1964, 704, 3533, 1519, 2979, 418, 3551, 1719, 2267, 380, 3169, 3162, 3283, 3716, 2693, 3098, 2626, 1923, 2754, 1907, 65, 3044, 1682, 3314]. **Mathematically** [2580, 1901]. **Mathematically-optimized** [2580, 1901]. **mathematicians** [1396]. **Mathematics** [79, 1184, 1930, 2328]. **MATLAB** [3626, 1294]. **MATOPT** [3284]. **Matrices** [807, 866, 1070, 870, 2130, 3291, 638, 2777, 3658, 366, 714, 2058, 2136, 3634, 462, 529, 316, 204, 476, 3043, 2320, 2695, 2888, 2310, 2807, 3062, 3149, 3165, 3223, 3379, 3464, 3477, 3593, 2251, 2852, 1921, 547, 2531, 321, 465, 1612, 250, 324, 1672, 1652, 349]. **Matrix** [1992, 865, 778, 857, 2736, 887, 1028, 3190, 3191, 3192, 516, 1821, 2068, 1696, 1697, 2006, 1757, 3054, 3409, 397, 564, 1341, 2196, 2689, 1395, 190, 2555, 1576, 1582, 2161, 352, 962, 3701, 379, 2298, 2371, 3043, 2833, 3215, 3282, 512, 657, 305, 3062, 3381, 234, 3347, 228, 3369, 485, 613, 3262, 332, 1966, 26, 270, 1039, 473, 575, 175, 2661, 2707, 1329, 1511, 452, 532, 2399, 1259, 3003, 1473, 654, 1947, 2204, 1439, 1816, 363]. **Matter** [1162, 1083, 1493, 1675]. **matters** [3585]. **Matula** [2205]. **maturity** [2277]. **maxima** [1069]. **Maximal** [1726, 179, 2866, 2959, 1298, 2122, 1239, 1186, 696]. **Maximally** [3293]. **maximization** [1879]. **Maximum** [1576, 1121, 1470, 810, 1147, 1120, 2815, 1095, 328, 2569, 1192, 398, 2260]. **may** [2207]. **McClelland** [2789]. **MCSCF** [1394]. **MD** [2624, 1283]. **Mean** [3259, 3100, 1780, 1948, 3099, 1001, 3665, 2348, 2561, 1766]. **Mean-based** [3259, 3100, 3099, 3665]. **mean-field** [1001, 2348, 2561]. **Means** [813, 1800, 1362, 3076, 3466, 3145, 1095, 687, 3462, 2904, 2046, 2081, 3024, 739, 961, 1571]. **measurable** [2329]. **measure** [1615, 2109, 335, 3273, 3472, 1657, 1503, 1954, 2177, 2199, 2313, 3377, 2065, 1558]. **measured** [3083, 1746]. **Measurements** [1079, 1095, 1204, 1539, 1767, 1784]. **Measures** [1070, 1066, 770, 1089, 746, 520, 597, 1369, 1370, 471, 480, 486, 3729, 93, 3347, 3366, 1812, 1041, 1667, 3049, 1622, 2667, 2179, 3444, 3469, 571, 3093, 653, 2315, 1774, 368, 432, 3452]. **Measuring** [2097, 3414]. **Mechanical** [890, 866, 928, 930, 1052, 799, 2787, 2705, 2514, 1971, 2412, 2397, 2406, 3542, 2364, 2153, 2383, 2649, 2408, 2533, 2715, 1613, 3305, 3718, 3058, 2233, 3688]. **mechanically** [2121]. **Mechanics** [1567, 888, 472, 2006, 2672, 3353, 2307, 187, 101, 2393, 610, 1758, 343, 1570, 2365, 2275, 2407, 2360, 2554, 194, 2509, 1076, 3491, 347, 389, 390]. **Mechanism** [903, 894, 2776, 2189, 3193, 2343, 2990, 1191, 1957, 118, 3036, 1995, 2917, 2752, 214, 3074, 3423, 1434, 983, 1360, 1522, 487]. **Mechanisms** [1849, 834, 3284, 2000, 3503, 19, 146, 2091, 1463, 1693, 246, 593, 695, 306, 2436, 1464]. **Mechanistic** [2254, 2905, 1335]. **mechanochemical** [3494]. **Mechanochemistry** [3684]. **Media** [874, 2732, 2247, 1618, 745, 2470, 2963, 3208]. **median** [1196]. **mediated** [2750, 1862]. **mediator** [2999]. **medical** [3292]. **medicine** [2580, 3720]. **Medium** [757, 845, 2724, 410, 2327, 745, 2484, 3615, 3102]. **MEDLA** [440]. **Melencolia** [3710]. **melting** [2993]. **melts** [310]. **membered** [2450, 2451, 2452, 3456, 3457, 3468, 1914]. **memberships** [2081]. **Membrane**

[880, 1159, 861, 2635, 2293, 1794, 1731, 2051]. **Membranes** [1055, 2167, 2588, 2929, 1402]. **Memoriam** [3511]. **memory** [2832, 3019, 3111, 3028]. **Menger** [2650]. **Menten** [2518, 2644, 2254, 2344, 2095, 1878, 1987, 3048, 2884, 2419, 1689, 2281, 1584, 3728, 2238, 2819, 3533, 2236, 487]. **Merrifield** [1223, 2949, 1575, 1186, 1264, 1230, 1109]. **Mersenne** [3076]. **mesh** [3565, 3575, 3397, 2480, 2339]. **meshes** [3361, 2339, 1677, 1436]. **Meshless** [3040, 1680, 3042]. **mesophase** [3387]. **Mesoscopic** [2793, 1795, 3387]. **meta** [2071]. **meta-analysis** [2071]. **metabolic** [2887, 2307]. **metaheuristic** [3696]. **Metal** [861, 3338, 3686, 1890, 3655, 2686, 13, 96, 3523, 2206, 2992, 2687]. **metal-insulator** [96]. **metal-organic** [1890]. **metallic** [1680, 1102]. **metallocene** [1981]. **metallofullerenes** [3317]. **metals** [96, 2931]. **metamaterials** [2957]. **methacrylic** [1530]. **methanation** [2845]. **methane** [1922, 1532]. **methanol** [3082]. **Method** [871, 763, 851, 1175, 625, 1079, 858, 1107, 3466, 1019, 780, 1154, 836, 772, 1140, 806, 874, 3355, 1065, 624, 3400, 1116, 902, 3138, 771, 754, 1137, 1084, 1161, 773, 906, 1306, 3639, 2463, 2373, 2060, 2029, 2118, 2178, 2253, 2410, 2322, 2544, 2524, 2549, 2472, 2662, 2691, 2709, 2938, 2908, 3039, 2991, 3116, 1797, 2538, 2757, 2759, 2663, 1352, 639, 36, 708, 3054, 174, 3709, 3086, 1692, 2764, 2734, 2746, 1280, 557, 1955, 261, 2016, 2043, 2879, 1226, 1256, 1291, 1362, 1762, 1948, 3543, 1736, 2751, 2922, 3353, 3155, 3330, 3111, 139, 3361, 675, 435]. **method** [1533, 2492, 113, 2075, 1891, 1156, 539, 231, 2998, 2490, 2872, 3299, 3312, 3606, 3708, 3691, 1229, 2298, 2299, 2371, 2372, 3456, 3457, 3468, 3325, 656, 3427, 1483, 2927, 1751, 2085, 2146, 2245, 3282, 3181, 3240, 2384, 241, 563, 3594, 1921, 3440, 3386, 1642, 1636, 2953, 3482, 3418, 1633, 1695, 1840, 1597, 2481, 3322, 2909, 3034, 3616, 2379, 221, 2480, 1587, 1568, 1626, 2215, 2105, 426, 446, 1954, 2339, 2419, 3264, 2633, 3163, 3231, 3242, 3335, 3378, 3480, 3539, 1651, 1836, 2847, 2856, 3109, 3040, 3141, 3682, 2770, 3253, 2694, 2897, 2896, 3227, 2904, 3008, 3450, 3633, 3513, 2903]. **method** [2047, 26, 2733, 2795, 3172, 3278, 3364, 3300, 3268, 3280, 3349, 3302, 3316, 3548, 3608, 1570, 2554, 3269, 2718, 2796, 3459, 1006, 2507, 3244, 2511, 2529, 166, 2145, 1482, 2213, 3267, 686, 683, 600, 572, 1647, 1535, 2057, 3150, 3235, 2954, 2284, 3412, 1386, 2558, 3435, 3101, 2232, 2333, 1678, 970, 1069, 1872, 3156, 3125, 3304, 3495, 3572, 2429, 653, 3136, 3139, 2779, 3239, 3573, 3197, 2380, 3199, 713, 1101, 1548, 1904, 2317, 2381, 2370, 2455, 30, 31, 2335, 2618, 2921, 3584, 1434, 451, 2930, 3370, 3274, 3266, 3249, 3611, 717, 730, 3689, 2528, 1862, 2241, 2530, 2769, 3283]. **method** [3716, 3622, 2768, 2868, 2204, 3279, 1821, 2050, 2022, 2258, 2563, 48, 1939, 1411, 963, 2135, 2720, 3160, 2302, 2723, 2774, 2648, 2854, 3592, 3724, 2914, 732, 2775, 2876, 350, 349, 1614, 389, 390, 3407, 2883, 1358, 2719, 727, 2594, 2655, 89, 733, 1478, 725]. **methodologies** [1508, 2033]. **methodology** [1527, 1526, 165, 2044, 3162]. **Methods** [755, 1114, 763, 764, 817, 752, 1078, 1105, 780, 806, 804, 1160, 758, 800, 863, 912, 959, 867, 889, 832, 3015, 1745, 1754, 1798, 1871, 2392, 2632, 2595, 2673,

2623, 1683, 3023, 966, 1559, 1479, 1527, 1526, 2647, 3018, 3031, 3108, 949, 957, 1632, 1735, 1860, 684, 978, 85, 483, 3118, 3117, 1139, 3132, 1064, 1206, 3673, 1277, 2478, 595, 3259, 3372, 1770, 3019, 3099, 3100, 2761, 2892, 2516, 1912, 2225, 121, 3676, 3564, 2848, 2110, 2283, 2893, 3674, 610, 2248, 3610, 2566, 1842, 965, 3519, 585, 3170, 1750, 84, 2778, 3084, 624, 1394, 2169]. **methods** [3714, 2143, 2334, 3026, 1381, 2763, 2894, 2244, 3107, 2645, 3739, 376, 964, 1098, 2024, 3191, 1525, 516, 967, 1099, 1540, 3194, 3569, 968, 3359, 3297, 3665, 554, 607, 637, 1355, 2098, 3405, 3210, 3081, 1409, 2331, 1528, 440, 3218, 3033, 2699, 2835, 3030, 2891, 3028, 2697, 2698, 2853, 1816]. **methoxyethanol/2** [3184]. **methvlamine** [469]. **Methyl** [2990, 3330, 3462, 3074]. **Methylated** [1134]. **methylation** [3422]. **methylene** [2085]. **methyltransferase** [1418]. **Metric** [827, 914, 791, 941, 984, 1288, 1370, 3234, 3505, 3703, 2805, 326]. **Metrics** [888, 441, 442, 443, 58]. **Mg** [1513]. **Micellar** [943]. **micelle** [1768]. **Micelles** [773]. **Michaelis** [2095, 2518, 2644, 2254, 2344, 1878, 1987, 3048, 2884, 1320, 2419, 1689, 2281, 1584, 3728, 2238, 2819, 2036, 3533, 2236, 487]. **Michaelis-type** [2036]. **Michalis** [3690]. **Micken** [3014]. **Mickens** [2880]. **micro** [2233]. **micro-electro-mechanical** [2233]. **microbioreactor** [1767]. **microdomains** [3387]. **microequilibrium** [670]. **microorganism** [1658]. **microporous** [2786]. **microreactor** [649, 3196]. **microscope** [440]. **Microscopic** [1990, 981, 1648]. **microseconds** [311]. **Microvia** [2353]. **microwave** [3675, 2487]. **microwave-assisted** [3675]. **Mie** [1972, 2468, 1266]. **Mie-type** [1972, 2468]. **Might** [3532]. **migration** [1334, 1562]. **mild** [2386]. **milling** [3494]. **Milovanović** [3666]. **mimicking** [1181]. **mind** [3154]. **minima** [560, 622]. **Minimal** [753, 1250, 1168, 800, 2260, 1158, 1311, 1696, 1697, 3493, 2000, 2778, 643, 1189, 2857, 1186, 1210, 554, 1819, 382, 1048, 1637, 976, 1063]. **minimax** [367]. **minimization** [2331, 3470]. **minimizing** [1499]. **MInimum** [1306, 1728, 1631, 1121, 3230, 1758, 3289, 1836, 1473]. **Minimum-uncertainty** [3289]. **Minkowski** [827, 1370, 2731, 3275, 3277, 3234, 443, 2555]. **Minkowskian** [3453]. **mirror** [2144]. **misbelief** [407]. **Misgivings** [666]. **mismatch** [2200]. **missense** [3638]. **missenses** [3629]. **mitochondrial** [1505, 2430]. **Mittag** [1026, 996]. **Mittag-Leffler** [1026, 996]. **Mixed** [1544, 2086, 2290, 1935, 656, 455, 3113, 2725, 1069, 2997, 3505, 459, 3556]. **mixed-entropic** [2086]. **mixing** [1049, 1243, 434]. **mixture** [1208, 3599, 3590, 219]. **Mixtures** [934, 2940, 1361, 2793, 1592, 3524, 1647, 2601]. **MLR** [940]. **MM-ER** [1534]. **MO** [721, 690, 1070, 1287, 1288, 1289, 1805, 1953, 2103, 2614]. **Mobilities** [845]. **mobility** [2832]. **Möbius** [2672, 1128, 206, 229, 172, 3013, 2692]. **Mode** [776, 3123, 2732, 3421, 249, 2013, 3435]. **Model** [750, 898, 861, 776, 1197, 1198, 926, 766, 1024, 902, 3395, 492, 1628, 1908, 2130, 2875, 1797, 3051, 3195, 918, 2669, 3286, 2829, 2185, 3401, 2311, 2254, 2095, 2434, 414, 470, 481, 491, 351, 193, 2202, 1395, 3337, 2152, 2114, 3410, 2291, 2445, 1878, 3258, 2571, 100, 3731, 3157, 2165, 2168, 319, 434, 1740, 3589, 3126,

12, 1686, 3455, 3711, 2998, 1213, 1935, 3526, 3298, 2048, 2049, 2451, 570, 3020, 2187, 3082, 3429, 1035, 1383, 1818, 2045, 202, 71, 2409, 1874, 2085, 3282, 1562, 1714, 1715, 3025, 1181, 3699, 120, 2744, 3668, 2227, 1515, 2361, 1497, 3386]. **model** [534, 53, 54, 2970, 2801, 2955, 58, 3041, 1299, 1503, 1954, 2259, 2419, 2700, 1428, 2219, 2941, 3055, 2244, 2281, 3633, 3403, 2306, 1723, 1724, 2946, 1717, 1841, 2073, 2155, 2295, 2515, 2874, 3001, 3046, 2208, 2094, 2285, 1734, 2087, 1204, 1504, 258, 288, 2038, 1332, 2113, 3523, 745, 2484, 2102, 3675, 3422, 185, 2353, 444, 2675, 1043, 2857, 3718, 647, 2246, 2979, 1512, 2157, 2123, 2470, 3667, 3552, 11, 3237, 1583, 230, 2921, 1195, 3518, 3611, 2978, 160, 3717, 537, 1573, 2787, 1839, 1594, 3169, 1823, 1601, 1879, 3098, 2626, 413, 2239, 2300, 3059, 3121, 2737, 3635, 2988]. **model** [2422, 2356, 2616, 2929, 3656, 3670, 3690, 1340, 1301, 1967, 2354, 2610, 3597, 1402, 1703, 1682]. **modelability** [3024]. **modeled** [338]. **Modeling** [1661, 943, 3196, 1800, 768, 3330, 1040, 2272, 1412, 2388, 1169, 1212, 775, 1824, 2036, 1781, 1925, 2262, 1170, 1532, 3236, 3615, 1767, 3208, 1508, 2964, 1245, 977, 2510, 3383, 1418, 2225, 3374, 3072, 202, 669, 2831, 2308, 2359, 2067, 3060, 1749, 2025, 1689, 2055, 2166, 2506, 2293, 3728, 2250, 2238, 2656, 3623, 3458, 1588, 1537, 2779, 3663, 2267, 1981, 2830, 2693, 1565, 1551, 1746, 3210, 2156, 2881, 2912, 1731, 2919]. **modelled** [3638]. **Modelling** [2240, 2220, 1897, 1782, 1922, 649, 828, 880, 1055, 1159, 1813, 815, 2624, 1928, 1853, 2710, 1531, 2141, 1404, 2046, 3158, 250, 2467, 2924, 3153, 3256, 2147, 1817, 261, 2976, 1536, 220, 2937, 3631, 3103, 1671, 972, 1509, 2955, 2621, 1693, 243, 2488, 1999, 2405, 1606, 3629, 3638, 525, 1794, 1821, 2022, 2258]. **Models** [940, 768, 790, 859, 929, 310, 1200, 1127, 1975, 846, 1337, 1018, 2514, 1971, 2412, 2905, 3713, 3247, 1401, 2762, 1243, 595, 2464, 2760, 1602, 3393, 2841, 2944, 1505, 2715, 339, 3448, 1384, 1229, 2517, 1334, 1377, 3661, 3417, 657, 1951, 138, 2588, 3726, 3397, 1194, 1303, 1775, 314, 313, 2894, 2583, 1613, 1584, 246, 33, 1985, 1990, 1404, 2609, 2638, 2637, 3327, 3376, 3024, 3194, 2347, 2561, 346, 3272, 3351, 614, 1411, 2754, 192, 2430, 2051]. **Moderate** [945]. **modern** [2111, 584]. **modes** [3415, 2308, 469]. **Modification** [1639, 2415, 2679]. **modifications** [665, 1759]. **Modified** [1556, 2445, 563, 771, 2835, 1956, 3193, 3489, 1963, 2110, 1671, 3072, 1320, 2388, 3726, 2143, 2334, 3026, 2415, 1212, 2529, 3267, 1824, 2036, 3394, 3423, 2232, 970, 1069, 3551, 3408, 607, 2618, 3211, 2931]. **modifier** [1796, 983]. **modulated** [2584, 2585]. **modulation** [2412]. **modules** [525]. **modulus** [981]. **Molar** [47]. **MOLCEN** [271]. **Molecular** [1970, 856, 1126, 2287, 928, 1030, 1070, 1066, 1370, 271, 3466, 2411, 1123, 962, 1021, 790, 791, 1187, 1083, 202, 1151, 266, 1065, 3067, 1336, 1138, 809, 783, 784, 1968, 1068, 846, 194, 3146, 302, 1168, 503, 1537, 1847, 1719, 1090, 1119, 3348, 2142, 1155, 2052, 3688, 2034, 2705, 580, 130, 673, 2032, 1258, 2074, 253, 1236, 2732, 2203, 1958, 2005, 1324, 681, 105, 520, 598, 1346, 1989, 1973, 2058, 2188, 2131, 2534, 2649, 3318, 3634, 471, 480, 581, 3532, 2420, 529, 335, 995, 416, 500, 1881, 3137, 1946, 2598, 1761, 1388, 3143, 1286]. **molecular** [3445, 980, 1447, 248, 46, 3334, 3035, 3417, 3727, 2026, 86, 56, 318, 1461, 1462,

3306, 1425, 2681, 278, 2575, 747, 426, 427, 2149, 1426, 1705, 1298, 1873, 1350, 1456, 1599, 1600, 402, 688, 1372, 45, 1852, 1041, 406, 705, 44, 43, 156, 439, 464, 490, 1440, 1399, 1960, 246, 3654, 3521, 2208, 3485, 3541, 3723, 437, 982, 1349, 1354, 1235, 1445, 1629, 1622, 1787, 1802, 1790, 2008, 2104, 2108, 2382, 2619, 1239, 2145, 2013, 1455, 2791, 704, 2857, 163, 2263, 3209, 164, 601, 1473, 526, 3537, 2192, 2175, 537, 2528, 2230, 1436]. **molecular** [2093, 1048, 385, 599, 1720, 3568, 1251, 106, 1342, 2655, 463, 545, 32, 583]. **Molecular-mechanics** [194]. **Molecule** [1021, 878, 873, 2240, 141, 2264, 1897, 1514, 2614, 2445, 2304, 531, 3526, 1769, 1181, 1477, 1197, 1198, 2149, 2127, 2126, 99, 3617, 2260, 1822, 577, 732, 2356, 3656]. **molecule-adapted** [2260]. **Molecules** [767, 848, 839, 1088, 1031, 893, 906, 1119, 1155, 2220, 472, 611, 2653, 1359, 168, 2343, 1556, 367, 2879, 142, 1393, 2435, 1890, 100, 113, 2513, 2496, 510, 659, 1366, 1471, 1595, 2099, 1244, 538, 3350, 2223, 1481, 1811, 2567, 167, 547, 355, 1001, 1587, 747, 643, 1189, 1828, 387, 1469, 314, 313, 125, 1895, 2306, 553, 315, 307, 172, 1645, 2269, 2301, 2270, 2345, 2432, 3623, 642, 70, 1980, 672, 533, 359, 199, 3052, 2352, 1844, 150, 3, 2323, 67, 1756, 35, 440, 461, 1998, 2277, 1251, 2685, 727, 734]. **Molien** [3296]. **Molnupiravir** [3631]. **Moment** [1049, 3377, 1153, 2397, 379, 2490, 1096, 2972, 2791]. **momenta** [3634]. **Moments** [2021, 72, 300, 1352, 3080, 1006, 2730, 601, 2350, 545]. **Momentum** [1171, 1060, 2034, 580, 1982, 2112, 2383, 1205, 1284, 1338, 1385, 1468, 1604, 944, 2132, 1812, 2551, 2527, 737]. **momentum-space** [580]. **monatomic** [3599]. **monic** [1233]. **Monitoring** [1020, 200]. **Mono** [872, 3659]. **Mono-Substitution** [872]. **monobromide** [1711]. **Monocyclic** [1011, 2415, 2679, 1332]. **Monod** [1310, 1195, 1594, 1254, 1231]. **monodimensional** [1615]. **monodisperse** [310]. **monoiodide** [2424]. **monolayer** [2705, 3618]. **monolayered** [1313, 1111]. **monomer** [1530, 539, 344, 2348, 1643]. **monomer-excimer** [539]. **monomer-monomer** [2348]. **Monomial** [780, 2900, 2898, 2899, 697]. **monophenolase** [1704]. **Monoradicals** [792]. **monostationarity** [3680]. **monosubstrate** [1786]. **Monotone** [1129, 3609]. **Monotonicity** [814, 2818]. **Monte** [3383, 455, 2947, 3035, 530, 2686, 1587, 1944, 2779, 3622]. **Morales** [983]. **Morita** [1413]. **MORPH** [1749, 2025, 2548]. **morphed** [2149]. **morphogenesis** [1625]. **morphology** [1918]. **Morrison** [3149]. **Morse** [608, 2879, 3343, 1963, 2227, 1065, 922, 1145, 1325, 1639, 1820, 406, 2360, 2336, 3289, 575, 3002, 2668, 2413, 2630]. **Morse-Type** [1145]. **Moshinsky** [2183]. **most** [2748, 3424, 1506, 2749]. **Mostar** [3561, 3148, 2942]. **motifs** [2200, 2919]. **motion** [2747, 951, 467, 500, 3324, 1966, 378, 359, 2779, 1410, 3210]. **motions** [310, 2013]. **motor** [704, 2857]. **Mottram** [922]. **Moulton** [3567, 3714, 3739]. **Mountain** [703]. **Mountains** [1992]. **movement** [704]. **Moving** [749, 2727, 3476]. **mp** [766]. **mp-Cut-HDMR** [766]. **MR** [1454, 2071]. **MRS** [2579, 2740, 3431, 3570, 3735]. **MS** [2369]. **MS-Windows** [2369]. **Mulitstep** [1754]. **Mulliken** [930, 1070, 1645]. **Multi** [1167, 772, 2970, 2379, 798, 1550, 1731, 2842, 3543, 3660, 2999, 1214, 3696, 2688,

3668, 3601, 2169, 2184, 2269, 2423, 3422, 1290, 2356, 3656, 2697, 2853, 3688]. **Multi-center** [1167]. **multi-component** [1214]. **multi-configuration** [2169, 2184, 2269]. **multi-derivative** [3543, 2697, 2853]. **multi-dimensional** [2688]. **multi-exponentials** [2842]. **multi-fractional** [3668]. **multi-invariant** [1290]. **multi-molecule** [2356, 3656]. **Multi-objective** [2970, 1550]. **multi-platform** [3422]. **multi-point** [3601]. **Multi-Scale** [772]. **Multi-scales** [1731]. **multi-step** [2999, 3696]. **multi-term** [3660]. **multi-tissue** [3422]. **Multi-variate** [2379]. **multi-walled** [3688]. **multi-way** [2423]. **Multicenter** [836, 917, 919, 1017, 721, 145, 1226, 971, 1246, 1471, 1603, 1737, 651]. **Multicolour** [614]. **multicomponent** [634, 3102, 1285]. **Multiderivative** [912, 3170, 968, 2098]. **Multidimensional** [1992, 2761, 1615, 2089, 1095, 559, 3408]. **Multielectron** [917, 1246, 1603, 1737, 3150]. **Multienzyme** [833]. **multiharmonic** [1538]. **multilayer** [1956, 1993]. **Multilayered** [1071]. **Multilevel** [2241]. **multilinear** [2089]. **multimedia** [1699]. **Multimolecular** [2378, 2540, 2547]. **Multinomial** [910, 1033, 2928, 2981, 1185]. **multiparameter** [1870]. **multipartite** [2209]. **multiphase** [3102]. **multiphoton** [2224]. **multiphysics** [1928]. **Multiple** [816, 3628, 2991, 438, 1094, 2901, 1807, 3344, 3602, 2739, 3259, 3439, 416, 528, 2482, 2960, 1568, 1626, 698, 696, 697, 1625, 2971, 2395, 3657, 2891, 3407, 3064, 25]. **Multiple-attribute** [3628]. **multiple-root** [3439]. **Multiplet** [3206, 3205]. **multiplets** [1454, 3697]. **multiplication** [353, 354]. **multiplications** [512]. **multiplicative** [685, 569]. **multiplicities** [2087, 2497]. **multiplicity** [2952, 2269]. **multiply** [1313, 1111]. **multiply-connected** [1111]. **Multipole** [1028, 1153, 1039]. **multipoles** [408]. **multipurpose** [1762]. **multiquantum** [322, 696, 697]. **multireference** [3421]. **multiresolution** [747]. **Multiscale** [1508]. **Multispin** [811]. **Multistage** [2215, 2549, 3006, 3005, 3044]. **Multistationarity** [660, 3079, 2096, 444]. **Multistep** [832, 3039, 2991, 2828, 3006, 3564, 3596, 3170, 3335, 2795, 3037, 3349, 513, 1540, 2954, 1528, 1549, 3592, 3724, 2994]. **multitrees** [38]. **multivariance** [2833, 2423, 2707, 1739]. **multivariant** [1194, 1303]. **Multivariate** [2878, 2022, 3385, 2397, 2390, 2204, 1879, 1810, 1821, 2050, 2258]. **multivector** [2959]. **multiverse** [2153]. **multiway** [2707]. **Murrell** [922, 1308]. **mutagenicity** [2902]. **mutation** [2290, 3638]. **mutitpoint** [3108]. **mutual** [2088, 2100]. **mutually** [1723, 1724]. **MX** [2753, 2948]. **Myoglobin** [3036].

N [2272, 2145, 1414, 2968, 1979, 3122, 1222, 953, 1296, 1260, 2641]. **n-diamond** [1979]. **N-particle** [1414]. **n-th** [3122]. **N-U** [2145]. **Nagumo** [2248]. **naive** [650, 2136, 3331, 1030]. **nano** [3641, 1378]. **nanoclusters** [2686, 1547]. **Nanocones** [1023, 1318, 1782, 3158]. **nanocrystalline** [1979]. **nanocrystals** [1546, 1543, 1544]. **nanoenvironment** [950]. **nanoflakes** [2164]. **nanofluid** [3669]. **nanojoins** [2557]. **nanomaterials** [2510].

nanoneedle [1441]. **nanoparticle** [2433, 2978, 3272]. **nanoparticles** [1817, 1545, 1996, 3654, 2296]. **nanoscale** [1567, 2779]. **nanosheets** [2965]. **nanoslit** [1001]. **nanoslit-pores** [1001]. **nanostructure** [1421]. **nanostructured** [2957]. **nanostructures** [2163, 2361, 2609, 3254]. **nanotori** [2965, 2375]. **nanotorus** [3540, 1209]. **nanotube** [492, 3540, 1813, 2802, 3515, 1428, 1432, 1822, 3688]. **Nanotubes** [3339, 1126, 892, 3647, 1680, 2070, 1258, 2074, 2965, 3734, 1359, 1782, 1922, 3196, 2167, 1617, 1518, 3090, 994, 3550, 3506, 2375, 2296, 2640, 3133, 1435, 3568, 2288]. **nanotubical** [2654, 2934, 2945, 3200]. **nanotweezers** [2102]. **nanowires** [2750]. **naphthalenophane** [629]. **naphthyridines** [1621]. **narcissus** [1237]. **narrow** [2850]. **native** [1847]. **Natural** [2731, 2458, 3463, 2782, 2984, 3275, 471, 2568, 3001, 2867, 2484, 2857, 614, 2731]. **nature** [1973, 2649, 2113, 90, 2599, 1907]. **Ne-** [1773]. **Near** [822, 2769, 2403, 1945, 2464, 3294, 2414, 96, 1918, 2840]. **near-polyhedral** [1918]. **near-symmetric** [2414]. **Near/far** [2769]. **Near/far-side** [2769]. **nearest** [1214, 26]. **nearly** [1681]. **necessary** [235, 660]. **neck** [1646]. **neck-like** [1646]. **Negative** [865, 408, 668, 2680, 3502, 2616, 350, 349, 1789, 1620]. **negative-equilibrium** [3502]. **Negatively** [382, 2519]. **neglecting** [1729]. **neighbor** [1214, 1461, 1462, 26, 3554]. **neighbor-excluding** [1461, 1462]. **Neimark** [3455]. **neither** [660]. **neoplastic** [3527]. **Nernst** [2293, 2347]. **Nested** [2696, 334, 1318, 456]. **Network** [1182, 33, 918, 3247, 3531, 529, 2535, 1887, 669, 3507, 3309, 16, 2973, 124, 3478, 2869, 1641, 433]. **network-based** [3507]. **Networks** [1126, 934, 1163, 1129, 1134, 3173, 2993, 3624, 3168, 3286, 2814, 1258, 2074, 2663, 1309, 2316, 3000, 1343, 2307, 1905, 1530, 2494, 2001, 2659, 304, 3352, 1886, 1887, 1888, 2193, 3445, 1700, 1902, 1605, 3433, 2682, 170, 2173, 2223, 1834, 1920, 2096, 586, 3579, 3347, 1425, 134, 1568, 1626, 2215, 2105, 1518, 1985, 2796, 3332, 3246, 1307, 1976, 2677, 3219, 3220, 1991, 2246, 2351, 131, 1663, 306, 2536, 1934, 1485, 1825, 2674, 2881, 3348, 2520]. **networks-AGDC** [2494]. **Neumann** [2519, 713, 2475]. **Neural** [934, 529, 1530, 2494, 2193, 669, 134]. **neutralization** [2069]. **neutron** [1932, 1675, 1691, 1925]. **Neville** [1082, 1674, 1927]. **new-phase** [712]. **newly** [3145]. **newly-developed** [3145]. **Newton** [1956, 2757, 2759, 3114, 3108, 3427, 937, 1873, 2763, 2904, 941, 2041, 1357, 1993, 3266]. **Newton-like** [3108, 2763, 2904]. **Newtonian** [2802]. **next** [26]. **NH** [2968, 3417]. **Ni** [1547]. **Niblack** [1636]. **Nice** [3179, 3248]. **Niederlinski** [3658]. **Nigam** [1636]. **Nikiforov** [3466, 2145, 3267]. **Nirmala** [3652]. **nitrate** [450]. **nitric** [2220, 3256]. **Nitride** [1010, 3647, 3540]. **nitrocubanes** [1838]. **nitrogen** [1441]. **NMR** [61, 3710, 1085, 1245, 3205, 3206, 3288, 3292, 3500, 3538, 3604, 3720, 3697, 816, 3583, 3475, 3661, 134, 507, 559, 662, 795, 1290, 631, 322, 459, 555, 615, 614, 696, 697, 811, 192]. **NMR-spectra** [3661]. **NNRTI** [3638]. **NNRTIs** [3627]. **NO** [953, 1296, 1260, 1582, 2053, 1806, 1080, 2924, 3153]. **noble** [2686, 2788]. **Nodal** [793, 2039]. **node** [1778]. **nodes** [1778, 1779]. **Noise**

[2252, 1443, 2072, 2431, 2579, 3066, 3288, 3500, 3538, 3604, 2242, 3405, 2616]. **Noise-assisted** [2252]. **noise-corrupted** [2431]. **noisy** [3582, 2608, 2794, 3021]. **nomenclatures** [171]. **Non** [492, 2658, 2158, 2010, 861, 1945, 3207, 866, 931, 2571, 1130, 838, 888, 1019, 539, 3606, 1164, 879, 1943, 2218, 651, 1410, 837, 1161, 3106, 3284, 2148, 2514, 2231, 2653, 2403, 2732, 2794, 2773, 2920, 1807, 743, 3004, 3315, 1804, 3226, 442, 443, 291, 529, 82, 3361, 1881, 3096, 3122, 3324, 2494, 1791, 3137, 1156, 3174, 736, 3627, 206, 587, 2961, 1995, 2985, 2913, 2973, 3369, 1626, 1758, 2628, 2505, 3227, 1861, 125, 1773, 2680, 1372, 1723, 1724, 1693, 3088, 2221, 1985, 3508, 2402, 175, 1624, 1622, 2382, 2484, 2013, 2046, 1519, 1677, 1684, 1837]. **non** [1844, 2806, 2921, 469, 739, 2267, 537, 2396, 3102, 1539, 2007, 646, 2881, 2745, 1278, 274, 1000, 3212]. **non-additive** [1624, 1622]. **Non-adiabatic** [1945, 2985]. **non-adjacent** [587]. **non-alternant** [206]. **non-autocatalytic** [1723, 1724]. **non-autonomous** [537]. **non-bipartite** [1000]. **Non-Boltzmann** [3207]. **Non-Central** [837, 2010, 1837]. **non-classical** [2267]. **non-commutative** [1804]. **Non-Commuting** [866]. **non-compact** [442, 443]. **non-constant** [3227]. **non-Darcy** [2484]. **non-dilute** [1807]. **non-Eckart** [2013]. **Non-equilibrium** [2571, 2403, 2382]. **non-Gaussian** [3324]. **Non-Hermitian** [2218, 1791, 1156, 3174, 2396, 646, 1278]. **non-homogeneous** [2046]. **non-isomorphic** [1539]. **non-isothermal** [3122, 2494, 2921, 3102, 2881]. **non-kinetic** [3284]. **Non-Linear** [861, 879, 2158, 931, 539, 651, 743, 3004, 3315, 3226, 529, 1881, 3137, 736, 3227, 1861, 1693, 3088, 2221, 3508, 2402, 1519, 2806]. **non-Lipschitz** [3212]. **non-local** [3369]. **Non-Markovian** [1410, 2913]. **non-mass** [1985]. **non-negative** [2680]. **non-nucleoside** [3627]. **Non-orthogonal** [3606, 125, 175]. **non-parametric** [2794, 2920]. **non-parametrically** [2773]. **non-polar** [2732, 3096]. **non-proline** [2961]. **non-PT-symmetric** [1019, 1156]. **Non-regular** [1164]. **non-relativistic** [1758, 1773]. **Non-rigid** [1130, 2653, 1844, 469, 739]. **non-selfadjoint** [2231, 2745]. **non-separable** [1837, 2007]. **Non-smooth** [2658]. **non-standard** [1677, 1684]. **non-steady-state** [291]. **non-stochastic** [1372]. **Non-superaromatic** [492]. **non-symmetric** [2514]. **non-uniform** [3106, 3361]. **non-unique** [1626]. **non-weakly** [2973]. **non-zero** [2628, 2505]. **nonadapted** [412]. **nonadiabatic** [955, 1577]. **nonautonomous** [1512]. **Noncentral** [917, 1870, 1050, 2035, 2078]. **nonclassical** [2704]. **nonclassicality** [2539]. **noncommutative** [1942, 262]. **Nonconvex** [1654]. **nondegenerate** [3123]. **nondiagonal** [527]. **nonequilibrium** [2224]. **nonequivalent** [2681]. **Nonexistence** [3257]. **Nonhomogeneous** [874]. **nonhydrogenic** [222]. **Noninteger** [920, 919, 1017, 1167, 854, 1027, 3486, 971, 1321, 1471, 1603, 1737, 1659, 1769]. **nonintegrability** [3321]. **Nonisomorphic** [264]. **Nonisothermal** [1202, 1175, 774, 1256, 1291, 1362]. **Nonlinear** [3184, 1034, 1013, 926, 775, 2989, 188, 3670, 3023, 1486, 718, 2901, 3118, 3117, 3713, 1362, 3259, 3687, 3099, 3100, 3439, 2501, 2483, 2456, 2760, 1748, 319,

2923, 2355, 3312, 1384, 1751, 2245, 1377, 1562, 1660, 2482, 1842, 3516, 2064, 3386, 3363, 2014, 2215, 2132, 3159, 3539, 3682, 3110, 2894, 2244, 3008, 3450, 1718, 2903, 33, 2718, 3459, 3559, 3244, 3147, 3669, 1824, 1386, 1781, 3533, 1677, 1684, 3281, 3376, 3304, 3495, 3572, 2470, 3112, 3359, 3573, 2475, 3249, 3398, 3279, 2525, 2471, 694, 64, 65, 2891, 3028]. **Nonlined** [920, 854, 1027]. **Nonlined-Up** [920, 854, 1027]. **Nonlocal** [1942, 3123, 2346, 3167, 3677]. **nonnegative** [2548]. **Nonnegativity** [1215]. **Nonorthogonal** [584, 446, 243]. **Nonoscillation** [709]. **nonparabolicity** [425]. **nonparametric** [2842, 2809, 3320, 3434, 536]. **Nonplanar** [1894]. **Nonrelativistic** [749, 1385, 1475, 437, 1407, 1414]. **Nonscreened** [919]. **nonstandard** [2880, 3014]. **nonsymmetric** [482]. **nonuniform** [3547, 1677]. **nor** [660]. **Nordhaus** [3143, 1854]. **norm** [1598, 2731]. **Normal** [2013, 818, 2526, 3415, 2390, 1601, 2300, 2792]. **normalised** [3233]. **Normalization** [574]. **Normalized** [1563, 204]. **Normalizing** [3648, 3545]. **Normed** [1523, 1809]. **Norms** [827, 3277, 2286, 2350]. **Nosé** [1083]. **Nosé-Hoover** [1083]. **notation** [32]. **notations** [2878]. **Note** [882, 807, 2266, 1051, 228, 3140, 819, 905, 602, 1376, 2002, 1183, 377, 28, 2228, 2177, 2313, 2159, 1228, 653]. **Notes** [466]. **notions** [1523, 1809]. **Novel** [1870, 842, 1808, 2555, 858, 3674, 751, 1106, 1372, 2234, 3047, 921, 2698, 1494, 207, 3731, 2944, 3483, 1255, 3627, 3036, 2035, 1846, 3446, 2139, 1497, 3616, 1503, 2679, 705, 1851, 1647, 3052, 3376, 2033, 2204, 2258, 1566]. **NR** [2295, 2489, 2515, 3001]. **Nuclear** [816, 1030, 1083, 836, 920, 1151, 854, 1027, 596, 785, 141, 2906, 2466, 1483, 1181, 2985, 1599, 1600, 1773, 465, 1398, 1482, 1261, 1455, 1365, 2911, 3362, 555, 614, 326]. **nuclear-attraction** [1261]. **Nucleation** [151, 2044, 2869, 2978, 3272]. **nucleation-growth** [2978, 3272]. **nuclei** [400, 2448, 2044, 596]. **nucleobases** [3654]. **nucleophilicity** [3128]. **nucleoside** [3627]. **nucleotide** [2257]. **nucleus** [2538]. **Number** [925, 41, 1125, 1178, 787, 1117, 429, 1236, 294, 37, 2823, 3250, 66, 122, 2131, 3557, 627, 1257, 2933, 1631, 83, 2629, 1383, 1366, 375, 3229, 265, 2569, 388, 1910, 228, 1429, 603, 2306, 74, 419, 2865, 994, 2031, 1473, 3214, 1263, 1438, 1249, 3133, 1732, 2107, 1727]. **numbering** [2205]. **Numbers** [1416, 1163, 1090, 1172, 1493, 2560, 213, 212, 445, 3557, 224, 50, 2217, 1321, 3270, 3336, 587, 508, 2205, 509, 1408, 123, 517, 998]. **Numerical** [2875, 1666, 842, 1114, 763, 764, 817, 481, 752, 2800, 3598, 3660, 3583, 1078, 1856, 1935, 1671, 736, 1097, 1057, 1994, 3567, 2807, 3165, 806, 965, 3650, 3355, 2955, 3653, 782, 1689, 3679, 3513, 3001, 1174, 2488, 1716, 3430, 1677, 1684, 758, 3552, 150, 3239, 1234, 771, 800, 912, 3695, 1911, 2116, 2641, 3704, 3705, 867, 889, 1867, 832, 3042, 1745, 1754, 1798, 1871, 2060, 2029, 1956, 2178, 2410, 2322, 2544, 2524, 2549, 2472, 2632, 2673, 2623, 2662, 2709, 1797, 966, 1559, 1479, 1527, 1526, 3722, 684, 3054, 3401, 1880, 1777, 2734, 1900, 2095, 2016, 2043]. **numerical** [2596, 3543, 3517, 3155, 3486, 338, 2937, 1687, 2110, 3025, 2566, 2384, 3464, 3593, 3170, 3363, 2738, 1633, 1695, 1840, 2778, 3084, 1597, 2798, 3725, 2611, 2480, 2105, 624, 2633, 2143, 2334, 2847, 3026, 2694, 3008, 3450, 3633, 2851,

3243, 2946, 1717, 2515, 2711, 2874, 3559, 964, 1098, 2024, 2507, 958, 2529, 1329, 1511, 2213, 2119, 967, 1099, 1540, 1864, 3595, 2333, 2405, 3281, 3327, 968, 3663, 3359, 2380, 3199, 607, 637, 713, 1101, 1357, 1548, 1904, 3467, 3584, 2930, 3677, 1839, 2799, 2687, 963, 2648, 2775, 1644, 3407, 2594, 1316, 1715, 1842, 3198]. **numerically** [3381]. **numerics** [1945]. **Numerov** [965, 1548, 2868, 963]. **Numerov-type** [965, 1548, 2868]. **nutrient** [1195, 1594, 1374]. **nutshell** [1433]. **Nyström** [806, 2334, 1541, 2699].

O [3641, 953, 1296, 1260, 498, 1018, 3663, 2641]. **OASIS** [92]. **object** [2309, 1989]. **objective** [2567, 2970, 2056, 1550]. **objects** [2012, 3428, 2243, 117, 183, 692]. **Obrechkoff** [3109, 3033]. **observability** [606, 662]. **observable** [1335, 1766]. **observation** [1749, 2025]. **observe** [1795]. **observer** [3348]. **Obstacles** [383]. **Obtain** [928, 870, 521, 2018]. **Obtained** [1016, 3479, 2786, 3074]. **Obtaining** [2990, 2369, 2854]. **occurring** [3681]. **octagonal** [543]. **Octahedral** [910, 2728, 2936, 1895, 2753, 2948]. **octan** [2940]. **octan-** [2940]. **octanol** [1551]. **octet** [1274]. **odd** [294, 3179, 3462, 2171]. **ODE** [2221]. **ODEs** [1891, 1234]. **off** [3459, 3406]. **off-step** [3459, 3406]. **offset** [3105, 3322]. **Ogilvie** [1308]. **oil** [3675]. **ol** [2940, 1976]. **Old** [870, 2463]. **Olender** [731]. **oligomeric** [2121]. **Omega** [1420, 1421]. **on-axis** [222]. **once** [399, 3380]. **oncology** [2255]. **oncolytic** [3098]. **One** [1113, 2939, 1050, 872, 2657, 1138, 748, 933, 1708, 825, 1727, 2278, 492, 1224, 2514, 2647, 2832, 2951, 746, 2249, 2879, 3413, 414, 470, 1277, 1868, 3383, 3353, 273, 283, 2715, 2820, 323, 2664, 2625, 3411, 1205, 1284, 1447, 1595, 1659, 1769, 1053, 2297, 3650, 2247, 1778, 251, 3679, 2126, 2718, 1612, 3435, 1488, 1569, 2627, 1907, 64, 1044, 1054, 1253, 356, 332]. **one-** [1868, 3650, 332]. **one-body** [1612]. **one-centre** [356]. **One-dimensional** [1727, 1224, 2514, 2832, 3413, 470, 3383, 2715, 2820, 323, 2297, 3679]. **One-electron** [1138, 746, 283, 3411]. **one-electronic** [251]. **One-Forms** [748]. **One-Parameter** [825, 64, 1044, 1054, 1253]. **One-range** [1050, 1205, 1284, 1447, 1595, 1659, 1769, 1907]. **One-sided** [1113]. **one-step** [3435]. **One-two** [1708]. **ones** [1067]. **only** [2809, 694]. **onset** [3590]. **onto** [3182, 1095, 2085, 1911]. **Open** [1151, 68, 77, 892, 1956, 581, 3000, 550, 2870, 1366, 1595, 336, 1349, 572, 1455, 3373, 518, 2987, 131, 2536, 1534, 1446, 1786]. **Open-Ended** [892, 2536]. **open-shell** [572, 1534]. **opening** [3514, 2041]. **Operation** [802]. **Operational** [1407, 1414, 2033, 2338, 3054, 3215, 3282, 3369, 3262]. **operations** [3532, 2396]. **operator** [3291, 2373, 673, 2231, 1984, 3599, 3634, 2985, 97, 332, 363, 2062, 26, 542, 1501, 2428, 1939]. **Operators** [1028, 1153, 409, 2397, 2406, 1804, 3598, 2468, 139, 140, 2748, 2556, 1216, 2062, 2680, 2365, 2275, 1039, 3566, 1382, 532, 715, 2749, 2195]. **Oppenheimer** [2148, 886, 2153, 1161]. **opposite** [3149, 3165]. **opposite-bordered** [3149, 3165]. **Optical** [3639, 1543, 1545]. **Optimal** [91, 2330, 2739, 416, 1881, 1686, 1924, 1653, 1592, 1799, 2921, 2233, 2340, 2891, 3022, 2901, 2995, 3117, 1800, 744, 367, 3602, 2386, 3449, 3372, 3439, 149,

3711, 2888, 2567, 3519, 2798, 3067, 3231, 1336, 2795, 2855, 3217, 3280, 3349, 1538, 2975, 3125, 3495, 3665, 3693, 1565, 1551, 1621, 1784, 3069, 3407, 2834]. **optimally** [500]. **optimisation** [2056]. **Optimization** [764, 1080, 1085, 740, 2636, 1013, 3403, 1959, 1676, 2431, 2651, 1931, 3315, 1874, 1842, 1497, 2970, 2055, 3421, 203, 1879, 2563, 1322]. **Optimized** [763, 764, 3538, 3570, 3720, 3697, 1426, 1139, 1901, 2580, 3604, 3006, 2110, 2283, 2017, 3440, 1597, 2935, 2909, 1773, 1525, 2213, 1535, 2954, 2844, 2050, 2914, 2816, 3657, 2255]. **Optimizing** [3696, 2216, 3675]. **optimum** [185]. **oral** [3527]. **orbit** [2341, 2906, 3541]. **Orbital** [846, 3489, 3233, 190, 3486, 318, 3319, 2117, 1350, 1456, 2867, 1269, 1235, 1624, 1629, 1623, 1787, 1802, 1790, 2213, 3569, 616, 1788, 2192, 3717, 106, 3499]. **orbital-communications** [1629]. **orbital-free** [3489]. **Orbitals** [836, 917, 920, 919, 1017, 854, 1027, 1119, 1155, 2287, 505, 362, 145, 3232, 971, 1321, 1379, 1246, 1338, 1385, 1483, 1468, 1471, 1475, 1447, 1595, 1604, 1603, 1737, 1814, 587, 1599, 1600, 1482, 946, 1459, 1460, 1261, 2660, 2780, 2810, 242, 1232, 2260, 3715, 1251]. **orbiting** [1567]. **orbits** [161, 377, 2023]. **Order** [755, 1114, 763, 764, 817, 827, 928, 977, 1361, 806, 800, 908, 830, 889, 2130, 1745, 2060, 2118, 2524, 2549, 2673, 2662, 2691, 2709, 2938, 2908, 2991, 3116, 1413, 702, 684, 3493, 2901, 2995, 3117, 2842, 2809, 3083, 3604, 1692, 1655, 2734, 2367, 722, 470, 1202, 408, 1287, 1288, 1289, 1805, 2103, 3372, 3660, 1176, 2922, 3439, 3404, 3517, 2483, 2760, 2892, 1912, 995, 121, 2170, 3483, 3504, 3676, 3122, 2893, 1225, 60, 2943, 3662, 1121, 1265, 1498, 3596, 3712, 2556, 3645, 3170, 547, 1695, 1597, 2935, 2960, 2849, 527, 3369, 3616, 2105, 2541, 2499, 2725]. **order** [2600, 2808, 3242, 3335, 3480, 3471, 3692, 3714, 3528, 2770, 2904, 3450, 3633, 3403, 1966, 2903, 3107, 2795, 2851, 2855, 3186, 3497, 3548, 3586, 3608, 3739, 2221, 2867, 3459, 3508, 3559, 1174, 2507, 1612, 2511, 3430, 652, 967, 1099, 2036, 3412, 509, 3101, 3595, 1561, 3125, 3509, 3603, 3572, 3569, 699, 2380, 3199, 554, 713, 1357, 1993, 2098, 2335, 2475, 3391, 3584, 3693, 2822, 3426, 3707, 2192, 1500, 1845, 3689, 3705, 3677, 2799, 2674, 324, 1541, 2868, 3081, 682, 2428, 3556, 646, 1084, 1528, 1549, 2720, 2971, 3187, 2723, 1772, 2648, 3592, 3724, 3510, 2775, 2994, 3732, 3407, 1062, 1201, 1314]. **order** [1217, 1771, 2719]. **ordered** [343, 1518]. **Ordering** [1575, 1172, 1637, 2705, 3634, 83, 643, 626, 173, 1376, 998]. **orderings** [2596]. **orders** [3198, 1838, 3688]. **Ordinary** [842, 1666, 1797, 1696, 1697, 2089, 2090, 2319, 2320, 2695, 2888, 3544, 1816]. **Organic** [1074, 872, 3338, 3484, 3686, 2832, 2646, 1890, 161, 1761, 54, 58, 2263, 3537, 1565, 1102, 2655]. **Organization** [2979]. **organometallic** [2197]. **Orientation** [1822, 2793, 219]. **orientations** [183]. **Oriented** [767, 44, 1403, 2677]. **origin** [1989, 2176, 3514, 562]. **origins** [2765, 1830]. **Ornstein** [3656]. **ortho** [2755, 2451]. **ortho-D** [2755]. **ortho-stereogenicity** [2451]. **Orthogonal** [3409, 1140, 911, 2286, 3606, 125, 175, 2179, 223, 242, 1941, 973]. **Orthonormal** [1014, 1205, 1321, 1284, 1338, 1385, 1468, 1475, 1604]. **oscillating** [2938, 2908, 1479, 3287, 3714, 2855, 1525, 2987]. **oscillation**

[718, 628, 3150, 2729]. **Oscillations**
[115, 410, 1985, 1733, 2291, 1794, 660, 1857, 1703, 1786]. **Oscillator**
[797, 475, 718, 3413, 3664, 3343, 2751, 100, 2872, 3329, 3526, 736, 2099, 3181, 2710, 2738, 2365, 2275, 2360, 2552, 3512, 3566, 2439, 3049, 3476, 2668, 452, 532, 3305, 2352, 519, 3021, 2792, 3222]. **oscillators**
[2445, 2642, 2847, 1538, 3289, 2429, 2413, 2604, 2698]. **Oscillatory**
[858, 3393, 3609, 2848, 3610, 2398, 235, 2868, 3571, 2699]. **Ostrowski**
[2501, 2456]. **Other**
[761, 1236, 978, 990, 1555, 3631, 60, 3618, 624, 2704, 306, 3068]. **OUR** [1204]. **outbreak** [3121]. **outer** [3424, 2324]. **outer-most** [3424]. **outlier** [1587]. **Outliers** [1634, 3047]. **output** [1788]. **output-reduced** [1788]. **Ovarian** [3538, 1245, 2072, 2579, 2702, 3292, 3431, 3604, 3697, 3735]. **ovary**
[2579, 2741, 2740, 3320, 3358]. **Overall** [847, 2088]. **Overcoming** [1213]. **overdamped** [3050]. **Overlap** [917, 1014, 1160, 1953, 190, 659, 1321, 1379, 1814, 1580, 1350, 1456, 946, 1459, 1460, 1491, 2260]. **overlapped**
[2226, 3066, 3500]. **overLApping** [1306, 1095]. **overlooked** [1064]. **Overview** [811, 2225, 2708, 3717]. **owning** [3635]. **oxalate** [3686]. **oxalate-based** [3686]. **oxalic** [1700]. **Oxidation**
[802, 894, 1170, 3196, 2355, 2631, 2641]. **oxide** [2220, 2871, 3590, 3641, 3256]. **oxide-based** [3641]. **oxides** [1069]. **oxidized** [1660]. **oximes** [2781]. **oxiranes** [2450, 3456, 3457, 3468]. **oxo** [1621]. **oxoimidazol** [1102]. **oxygen** [3196, 2762, 1545, 3072, 1689, 970, 3635]. **oxyl** [1102]. **oxysulfates** [2495]. **Ozawa** [1729]. **Özcan** [1483]. **ozone** [2873, 200, 1360]. **Öztekin** [1483].

P [2785, 2845, 3325, 953, 1296, 1260, 3335, 3480, 3300, 3316, 3199, 111, 755, 817, 1928, 637, 211, 1634]. **P-FAIMS** [1928]. **P-graphs** [2845]. **P-stable** [3325, 3335, 3480, 3300, 3316, 3199, 817, 755, 637]. **package** [2923, 1294]. **packed** [1999]. **packed-bed** [1999]. **packet** [2630, 2703]. **packets** [3343]. **Packing** [767, 3180, 1991, 611, 149, 323, 2870, 553, 3357, 3254, 3133]. **packings** [602]. **Padé** [1085, 1139, 1453, 1454, 2254, 2255, 2431, 2608, 2579, 2602, 2794, 2702, 2809, 2967, 3083, 3320, 3358, 3735, 2854]. **Padé-based** [1139]. **Padé-optimized** [2255]. **PageRank** [2059]. **pair**
[2180, 2828, 1869, 2815, 2943, 1424, 1747, 2324, 2798, 2143, 2334, 3026, 2855, 583, 2844, 961, 2803, 2816, 2834]. **pair-density** [1869]. **pairing**
[422, 206, 103, 209, 551, 583, 285]. **pairs**
[2859, 3498, 3179, 2750, 1985, 223, 2522, 3248]. **pairwise** [1407, 1414]. **Pais** [3021]. **palladium** [2398]. **Palmer** [2309]. **pandemics** [3642]. **Pandey** [1118]. **Pantea** [1485]. **Paper** [754]. **papers** [3621]. **para** [2755]. **para-H** [2755]. **Parabolic** [1751, 3106, 2923, 3034, 3459, 3101, 3197, 3467]. **paradigma** [694]. **Paradox** [1124, 690, 2466, 3164, 1775, 1947]. **paradoxa** [3314]. **Parallel** [483, 1933, 1927, 2158, 255, 456, 1425, 3556, 1547]. **parallelogram** [1390, 1965]. **parallelogram-like** [1390, 1965]. **paramagnetic** [1722]. **Parameter**
[1912, 1444, 825, 3116, 2647, 1395, 2408, 2533, 3601, 1653, 1538, 3595, 2979,

3391, 3613, 2050, 64, 1044, 1054, 1253, 1620, 1727]. **parameter-dependent** [2408, 2533]. **Parameter-free** [1444]. **parameter-robust** [3595]. **parameter-space** [2979]. **parameter-uniform** [3601, 3391]. **Parameterized** [914, 984]. **Parameters** [1175, 928, 1118, 3106, 2940, 3284, 1352, 3577, 2557, 1362, 1277, 1313, 3696, 14, 1957, 2778, 3041, 1749, 2025, 992, 1325, 1705, 1639, 1820, 672, 185, 1588, 3625, 3197, 1473, 1839, 2839, 1867, 1193, 3657, 2891]. **Parametric** [1905, 1013, 2794, 2920, 3358, 1202, 2501, 2456, 2760, 231, 3107, 3267, 3028]. **parametrically** [2773]. **Parametrization** [768, 3507]. **parking** [214]. **part** [2934, 2945, 3200, 2397, 2406, 2160, 2161, 2162, 1886, 1887, 1888, 2126, 1386, 3722, 763, 764, 978, 3205, 3206, 3320, 3358, 2319, 2320, 1741, 305, 723, 724, 2127, 513, 514, 593, 2098, 594, 933]. **Partial** [977, 1361, 1214, 2591, 3053, 1243, 3404, 2299, 2372, 656, 3725, 2379, 1564, 2399, 3119, 1838, 73, 3197]. **partial-cycle-index** [2299, 2372]. **partial-wave** [2379]. **Partially** [796, 707, 3532, 621]. **Particle** [2148, 2188, 811, 2180, 2068, 2373, 549, 2712, 2672, 951, 2665, 2101, 2362, 2519, 1780, 3374, 2727, 2913, 3730, 1812, 2047, 3354, 3469, 1332, 2113, 3733, 1408, 1407, 1414, 2630, 1981, 2787, 2926, 3210, 749, 1939]. **particle-in-a-box** [1812]. **particle-reinforced** [3374]. **Particles** [1149, 2964, 3132, 3503, 3576, 3542, 434, 2820, 2793, 1338, 1918, 712, 1727]. **particular** [1312, 1772]. **Partition** [1268, 827, 2918, 1187, 2797, 2306, 2023, 479, 3207, 2314, 3664, 1288, 2751, 2872, 1388, 538, 2864, 1613, 199, 3254, 1551, 3133]. **partition-of-unity** [2314]. **partitional** [525]. **partitioned** [2150, 2794, 363, 979, 2024]. **Partitioning** [978, 1142, 801, 190, 566, 661, 933, 2403, 2154, 121, 279, 1864]. **partner** [3628]. **partners** [2144]. **parvalbumin** [2947, 2919]. **Pascal** [37, 1213, 587]. **passive** [745]. **Passivity** [939]. **Passivity-Based** [939]. **paste** [1003]. **patches** [2622, 1416, 2414]. **Path** [3664, 402, 754, 1472, 666, 731, 1439, 111, 211]. **Path-Following** [754, 666]. **path-Zagreb** [1439]. **paths** [431, 81, 182, 723, 724, 1836, 2788, 280]. **Pathways** [937, 2000, 2644, 2887, 3086, 424, 2845, 3529, 578, 1335, 306, 697]. **patients** [3631]. **Pattern** [1175, 3726, 3690, 2875, 2724, 3103, 1740, 944, 2980, 3454, 1000]. **Patterns** [818, 2278, 3484, 2124, 3247, 3583, 3557, 227, 296, 1605, 1760, 1718, 104, 1405, 1823, 2988]. **Pauli** [2180, 1452]. **PB** [3001]. **PBB** [2147]. **PCP** [1664]. **Pd** [2290]. **PDE** [1045]. **PDEs** [3565]. **PDF** [1179, 1214]. **peak** [2842, 1069]. **peaked** [2684]. **peaks** [3066, 3500]. **Pecka** [940]. **Pedagogical** [456]. **pediatric** [2651]. **Pekeris** [2145]. **Pekeris-type** [2145]. **penalized** [2142]. **Pendant** [1109, 3470, 1120]. **pendent** [1270, 1575, 1264]. **Peng** [2931]. **penta** [2139, 2251]. **penta-diagonal** [2139, 2251]. **pentachains** [1146]. **pentadiagonal** [3224, 3062, 1921, 2531]. **Pentagonal** [2609, 3694, 2771, 2783]. **pentagons** [3248]. **pentameric** [1975]. **pentangle** [2574]. **Peptide** [1934, 394, 2961, 3090]. **Percolation** [197, 1402, 3429]. **Perelomov** [2552]. **Perfect** [1025, 1122, 152, 147, 2606, 2783, 787, 1199, 320,

627, 1326, 1480, 1510, 1211, 74, 419, 508, 3063, 2703, 2640, 1489, 2958]. **Perforated** [1055]. **Performance** [2705, 1615, 3194, 1436]. **peri** [2613]. **peri-condensed** [2613]. **pericondensed** [1218]. **pericyclic** [524]. **perifusenes** [273]. **Periodic** [1552, 826, 3094, 2986, 2503, 1646, 181, 80, 3393, 3487, 304, 1244, 170, 3334, 2401, 3477, 3499, 3243, 3276, 3569, 2822, 3518, 3068, 3128, 382, 1374, 3218, 1293]. **periodical** [2938, 2908, 2855]. **periodically** [1356, 1310, 1373, 1276, 1240, 1317]. **periodicity** [2979, 1969]. **Peripherality** [3352]. **Permanence** [1564, 1512, 1301]. **permanent** [462]. **Permanental** [899]. **permanganate** [1700]. **permanganate/oxalic** [1700]. **permeation** [1402]. **Permutation** [850, 2907, 2936, 3145, 269, 2142]. **Permutation-Group** [850]. **Permutational** [146, 1461, 1462, 512, 555]. **permutations** [2804]. **peroxide** [3258]. **peroxides** [2221, 2155]. **peroxidic** [1592]. **perpendicular** [3671]. **Perron** [1748]. **Persistence** [3351, 1886, 1887, 1888]. **persistent** [1699]. **personal** [2962]. **personalized** [2580]. **Perspective** [1030, 1490, 3558, 2136, 3535, 2089, 2162, 510, 3643, 1448, 3491]. **pertaining** [3011]. **pertinent** [615]. **Pertubative** [3382]. **Perturbation** [2276, 2490, 797, 725, 728, 3086, 3576, 397, 564, 334, 1804, 1796, 1987, 416, 2748, 2998, 3181, 3240, 1750, 1001, 2849, 527, 2215, 2407, 2439, 683, 3139, 2618, 1195, 1240, 1862, 2749, 2563, 2135, 2236, 560, 89, 215, 733, 1478, 671]. **Perturbations** [908, 2741, 962]. **perturbatior** [470]. **perturbative** [2985]. **perturbed** [3106, 3565, 3361, 468, 3712, 3594, 2064, 3363, 3034, 3397, 3601, 3725, 3681, 2847, 1677, 1684, 3101, 3595, 3197, 3391, 3467, 3695, 2241, 2616, 89, 215]. **pesticide** [3622]. **Petersen** [2653, 3700]. **Petrovskii** [2146]. **Pfaffian** [2950, 3013]. **PFLR** [1444]. **pg** [1456]. **pH** [3249]. **Phase** [3009, 3087, 3400, 3471, 3141, 3152, 2024, 3416, 771, 800, 1011, 3123, 1745, 1754, 1798, 1871, 2060, 2029, 2118, 2178, 2253, 2392, 2410, 2322, 2544, 2524, 2549, 2472, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 2938, 2908, 3039, 2991, 1559, 3493, 2734, 2746, 2479, 3006, 3130, 3504, 2815, 2893, 3137, 2684, 3325, 3089, 1700, 3662, 3012, 3596, 2566, 3005, 1840, 2778, 3084, 1597, 2798, 2909, 2910, 2044, 3264, 2633, 3131, 3163, 3231, 3242, 3335, 3378, 3480, 3692, 2856, 3061, 3077, 3253, 2198, 2679, 2733, 2855, 3037, 3172, 3186, 3217, 3243, 3278, 3364, 3300, 3073, 3268, 3280, 3349, 3497, 3548]. **phase** [3586, 3608, 2507, 2301, 2497, 2511, 2690, 1405, 542, 712, 2102, 3063, 127, 2263, 3119, 561, 1408, 3569, 2844, 989, 2380, 554, 1904, 2098, 2317, 2381, 2370, 2455, 1407, 1414, 2338, 2930, 1766, 3370, 3426, 1532, 3689, 2530, 2769, 2926, 3092, 3081, 3414, 1411, 1528, 1549, 2971, 3160, 3187, 3218, 2648, 3044, 3592, 3724, 2803, 2699, 2994, 3030, 2816, 1711, 2698, 3064, 3134, 2594]. **phase-equilibria** [2301]. **Phase-Fitted** [771, 3081, 2698]. **Phase-Fitting** [3400, 3471, 3493, 3504, 3662, 3596, 3378, 3480, 3692, 3364, 3300, 3497, 3548, 3586, 3608, 3370, 3426, 3689, 3592, 3724]. **Phase-Lag** [800, 1745, 1754, 1798, 1871, 2060, 2029, 2118, 2178, 2253, 2392, 2410, 2322, 2544, 2524, 2549, 2472, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 2908, 1559,

2734, 2746, 2893, 2566, 1840, 2778, 3084, 1597, 3264, 2633, 3242, 3471, 3253, 2733, 3172, 3186, 3243, 3278, 2507, 2511, 2380, 554, 1904, 2098, 2317, 2381, 2370, 2455, 2930, 3426, 1528, 3160, 3187, 3218, 2648, 3030, 2594]. **phase-shift** [554]. **Phase-space** [3009, 3416, 1408]. **phase/entropy** [2497]. **Phased** [1832, 1831]. **phases** [2270]. **phasor** [2504]. **Phenomena** [794, 802, 2785, 1917, 2097, 1664]. **phenomenological** [114, 1962, 60]. **phenomenology** [2198]. **phenomenon** [1906, 2963]. **phenothiazine** [1671]. **phenyl** [2492, 1976, 3136]. **phenylene** [1753]. **phenylenes** [1112, 3166, 2966, 1201, 1217]. **philicity** [3485]. **phonon** [3334]. **Phosphate** [798]. **Phosphocholine** [2773, 2794]. **phosphocyclopentadiene** [2208]. **Phospholipase** [1067]. **Phospholipidic** [856, 673]. **phosphorene** [3721]. **phosphorescence** [2404]. **phosphorylation** [3680]. **photo** [2631]. **photo-Fenton** [2631]. **Photochemical** [845]. **Photodetachment** [3424, 2519]. **photodissociation** [1522]. **photolysis** [2873, 1577]. **photon** [2739]. **photonics** [1405]. **photosynthetic** [2252]. **Phylogenetic** [1846, 1557, 2234, 3219, 3220, 1558]. **phylogeny** [2696]. **Physical** [915, 1127, 3553, 2638, 2637, 3327, 3376, 2265, 2442, 2601, 2133]. **physically** [1312]. **physico** [3577]. **physico-chemical** [3577]. **Physicochemical** [3625, 317, 3346, 1542]. **Physics** [1078, 1683, 2696, 1736, 9, 3408, 3741, 696, 697, 3283, 3716, 552]. **phytoplankton** [1512]. **Pi** [15, 876, 329, 1145, 956, 1112, 1218, 3265, 1140, 751]. **Pi-Electron** [15, 876, 329]. **pi-electrons** [956]. **pictorial** [30, 31]. **picture** [3416]. **pictures** [1004]. **pie** [3474]. **Piecewise** [2022, 2258, 1496, 2204]. **piecewise-linear** [1496]. **piezoelectric** [3647]. **pig** [350]. **Pina** [1130]. **pioneering** [3647]. **Pipek** [3511]. **Pisanski** [2768, 2846]. **Piskunov** [2146]. **Pitaevskii** [1097, 3359]. **pitch** [3387]. **Pitfalls** [2864]. **Pivotal** [3580]. **Planar** [2190, 2542, 2784, 1995, 1911, 2116, 2561, 734, 571]. **Planck** [2347, 3262, 624, 2293, 2405]. **Plane** [945, 818, 2374, 1000]. **planes** [2961]. **plankton** [1725, 3635]. **plankton-oxygen** [3635]. **plant** [2085]. **Plants** [1080]. **plasma** [3408]. **plasminogen** [1191]. **plasmon** [2957]. **platform** [3422]. **platforms** [483]. **platinum** [3590, 1551]. **Platonic** [1524, 1709, 1755, 1376]. **plausible** [2235, 2182]. **played** [1976]. **plot** [2504, 1064]. **PLS** [2831]. **Plus** [768, 401, 1870, 1556, 3178, 3447, 1241, 2035, 1895, 671]. **pockets** [2039]. **Podolsky** [1052, 1124, 3164]. **Poincaré** [2005]. **Point** [99, 770, 3406, 1165, 1933, 2158, 3345, 329, 633, 3432, 3115, 1989, 2058, 1915, 2109, 2188, 2466, 2490, 1328, 2298, 2371, 3519, 3306, 3601, 3681, 747, 3166, 2864, 183, 345, 692, 2295, 1540, 3045, 592, 2157, 1290, 2389, 3695, 1670, 644, 2471, 2805]. **point-clouds** [3432]. **Point-Group** [770, 2490]. **Point-Group/Subgroup** [770]. **point-like** [2466]. **point-sets** [1290]. **point-source** [2157]. **points** [2154, 2478, 1873, 119, 2041, 3435, 223, 1601]. **poisoning** [3082]. **Poisson** [2837, 3126, 2297, 2293, 2347]. **Pol** [3198, 2242]. **polar** [2732, 3648, 3096, 3035, 1001]. **polariton** [2957]. **Polarity**

[1561, 2871, 1457, 1458, 2966]. **polarizability** [3068]. **polarizable** [1874]. **polarization** [2208]. **Polarized** [2391, 2130]. **poles** [2741, 3451]. **pollutant** [2525]. **pollutants** [2646]. **polluted** [1515, 1584]. **poly** [1753, 1671, 3001, 3093]. **poly-butadiene** [3001]. **poly-phenothiazine** [1671]. **Pólya** [348, 2237, 109, 2546]. **polyacene** [1828]. **Polyacenes** [1169]. **polyaniline** [2388]. **polyaniline-modified** [2388]. **polyatomic** [3599, 2445]. **polyazulenoids** [2592, 2692]. **polybasic** [670]. **polybenzenes** [83]. **polybutadiene** [2711]. **polycarborane** [2037]. **polychlorobiphenyls** [3458]. **polycube** [74]. **polycubes** [257]. **Polycyclic** [933, 978, 2237, 360, 952, 3075, 3632, 2190, 2933]. **polycyclics** [31]. **polyelectrolyte** [2235, 2182]. **polyene** [30]. **Polyenes** [868, 1332]. **Polyethylene** [878, 873]. **polygonal** [2003]. **Polyhedra** [1089, 1654, 2378, 2540, 2547, 2443, 2665, 3634, 2411, 5, 22, 157, 1495, 381, 1376]. **Polyhedral** [3560, 770, 1268, 2004, 2020, 2172, 2918, 2862, 2053, 1524, 1709, 1755, 2059, 1883, 2543, 2972, 1712, 2171, 1918, 1726, 1806]. **polyhedron** [2572, 2689, 2020]. **polyhex** [1420, 112]. **Polyhexes** [238, 82, 227, 147, 81, 182, 336, 1221, 236, 1249, 1345]. **Polyhexes*** [1012]. **polyinositols** [2363]. **polylactic** [1951]. **polylogarithmic** [3144]. **polymantanes** [83]. **polymer** [1508, 261, 1401, 499, 3676, 3324, 1924, 304, 118, 1412, 310, 2682, 170, 535, 3539, 1441, 1212, 1404, 1824, 710, 159]. **polymerase** [2998]. **polymeric** [100, 1402]. **polymerisation** [2801]. **polymerization** [1040, 344, 1981, 1643]. **Polymers** [774, 3392, 198, 1530, 339, 669, 2009, 16, 252, 7, 1969, 346, 2693, 2340]. **Polynomial** [1015, 1855, 1060, 2351, 3168, 2866, 1393, 2435, 2268, 3535, 1420, 1421, 107, 1498, 1883, 2767, 28, 1469, 1752, 2718, 303, 3508, 76, 237, 104, 8, 358, 1650, 1977, 2956, 34, 35, 671]. **Polynomials** [836, 855, 911, 899, 57, 85, 3481, 3409, 3737, 3734, 3736, 3648, 2952, 21, 3713, 952, 3075, 3632, 1978, 2304, 2286, 1419, 2190, 1753, 2664, 2625, 1507, 170, 2066, 1760, 72, 5, 29, 10, 2390, 3221, 3328, 1712, 2171, 3213, 205, 3274, 973, 1233, 2769, 2350, 1272, 1435, 300, 2958, 489]. **Polyomino** [1148, 1910, 2122, 1203, 1611, 2606, 1783]. **Polyominoes** [177, 1760]. **polyominos** [2377, 2950, 2107]. **polypeptide** [438, 195]. **polypeptides** [3071]. **polyphenacenes** [1978, 1507, 998]. **polyphenols** [1537]. **polyphenyl** [1492]. **Polyradicals** [792]. **polyrex** [181, 63]. **polytropic** [2806]. **polyynes** [1293]. **Ponec** [940]. **pool** [2343]. **Pople** [1914]. **Population** [930, 830, 722, 2131, 2860, 3337, 1533, 3312, 3244, 1583]. **populations** [2131, 125]. **pore** [1897, 2085]. **pores** [1001, 3236]. **porous** [1646, 1320, 2247, 2067, 745, 2484, 3533, 2963, 3615, 3102, 1672, 1652, 3208]. **porphyrins** [1688]. **Port** [2881]. **Port-Hamiltonian** [2881]. **Portion** [1118]. **Pöschl** [3323, 417, 2671]. **posed** [2057]. **Posetic** [1134]. **posets** [474, 1365]. **Position** [2112, 1247, 1812, 1165, 2383, 1604, 3080, 2551, 2527, 737]. **Position-dependent** [1247, 1165]. **Position-momentum** [2112]. **Positional** [191]. **positions** [2842, 2088, 2100, 987]. **Positive** [3587, 408, 1679, 3228, 3433, 3386, 2925, 2813, 3649, 2093, 2249, 3507, 3579, 2559, 2062].

positiveness [1215]. **Possessing** [1158, 1588]. **possibilities** [3272]. **possibility** [2206]. **Possible** [857, 2991, 3273, 3389, 3651, 589, 3485, 670, 3615, 2994]. **Postcript** [209]. **posteriori** [3712]. **postulate** [2383, 494]. **postulates** [20]. **Potential** [943, 1085, 3115, 2817, 113, 924, 1021, 937, 1171, 1132, 723, 724, 1065, 879, 844, 860, 923, 932, 1015, 1135, 1145, 1237, 835, 840, 841, 945, 3395, 881, 773, 906, 727, 2180, 954, 1870, 1982, 2032, 1972, 2231, 1877, 707, 415, 1901, 2608, 3735, 3577, 1280, 1556, 1494, 1514, 3646, 2016, 2043, 2879, 981, 3323, 1393, 3232, 2101, 2304, 275, 2765, 3466, 1963, 3056, 3178, 3487, 3126, 1156, 3010, 3313, 3447, 3402, 3526, 1545, 3553, 1665, 1241, 1882, 971, 1769, 2099, 1133, 2727, 2227, 256, 2077, 3418, 108, 2149, 3308, 992, 1308, 1325, 1521, 1469, 1639, 1820, 1826, 1983, 1836]. **potential** [1873, 2941, 3403, 3563, 3605, 3562, 345, 2554, 2336, 2713, 473, 548, 575, 2056, 2214, 3295, 3276, 3444, 3425, 676, 1612, 2668, 1635, 1980, 2145, 3267, 2079, 3251, 3290, 683, 3394, 3045, 3527, 573, 1944, 418, 1344, 2352, 3371, 136, 2211, 1266, 1271, 417, 1407, 1414, 2630, 2840, 3333, 2007, 482, 560, 622, 2671, 1742, 2078, 2743]. **Potential-Energy** [924, 3526]. **Potentials** [1019, 917, 919, 922, 762, 1087, 837, 2034, 1224, 1870, 3129, 2514, 2538, 1972, 2010, 1556, 2203, 1958, 2005, 2986, 1973, 2751, 2468, 2872, 1050, 1659, 1769, 2384, 1481, 1247, 2681, 2349, 3002, 2144, 2439, 3425, 2668, 2113, 2201, 478, 418, 2429, 1837, 2530, 522, 560, 622, 1278, 1614, 671]. **Potentiometric** [1159]. **powders** [2085]. **Powell** [638]. **Power** [2164, 840, 841, 3587, 3023, 36, 2397, 2309, 996, 2731, 3520, 2812, 14, 2939, 1038, 2319, 3079, 3507, 3433, 128, 1983, 2925, 406, 2987, 2813, 3649]. **power-law** [2939, 3079, 3507, 2813]. **powered** [2779]. **powerful** [2701]. **powers** [2952, 2124, 2861, 2898, 2021, 2310, 2730, 452, 2023]. **PPP** [174]. **PR** [1746, 2229, 2385]. **Practical** [331, 564, 3418, 1901, 1288, 1953, 1375]. **pragmatic** [3699]. **pre** [2829, 1765, 3348]. **pre-diagnostic** [2829]. **pre-equilibrium** [1765]. **pre-filter** [3348]. **precise** [3154]. **precision** [2614, 1582]. **precursor** [664]. **precursory** [3387]. **Predict** [1046, 2705, 2340]. **Predicting** [168, 3373, 1838, 2883, 3340, 92]. **Prediction** [1067, 1768, 164, 3024, 91, 1530, 186, 2902, 2193, 3427, 1200, 1634, 2073, 2489, 3523, 2263, 3506, 3612, 1934, 2323, 2233, 3622, 3613, 1550, 134]. **predictions** [726, 128]. **predictive** [128]. **Predictor** [1099, 2524, 2472, 3673, 2213, 967, 2380, 2930]. **predictor-corrector** [2524, 2472, 3673, 2213, 967, 2380, 2930]. **Preface** [1415, 959, 1093, 1529, 1077]. **preferencs** [196]. **preparation** [2055]. **Preprocessing** [921]. **Prescribed** [1168, 1090, 1270, 1778, 1779, 1264, 1063]. **Presence** [926, 2278, 3738, 2072, 3303, 3451, 3589, 1225, 2235, 2182, 2426, 1723, 1724, 2404]. **presentation** [2225]. **Preservation** [2387]. **preserved** [3279]. **preserving** [2804, 3265, 3062, 3645, 2531, 3528, 3588, 2897, 3732]. **Press** [552]. **pressure** [3590, 2588, 3060, 2717, 406, 3506]. **pressures** [1194, 1303]. **PREVTH** [2898, 2899, 2899]. **Primary** [1141, 2071, 1557]. **prime** [83]. **primes** [3375]. **primitive** [944]. **Principal** [428, 749, 1285, 744, 1962, 1321, 2177, 2199, 2313, 2065]. **Principle**

[1047, 783, 3720, 3465, 2176, 319, 453, 510, 3525, 3424, 3655, 3065, 1685, 1648, 2545, 307, 3088, 513, 514, 593, 2056, 1452, 1790, 2836, 3154]. **Principles** [1335, 440]. **printing** [3222]. **prismane** [2048, 2049]. **Probabilistic** [2397, 2406, 2504, 2319, 2320, 2695, 2888, 2900, 1770, 3258, 1961, 1962, 2090, 2160, 2161, 2162, 2898, 3544, 2899]. **probabilities** [121, 2040, 623, 125, 1623, 1790, 1766, 1988]. **Probability** [1113, 1179, 940, 1070, 3241, 1260, 1198, 1626, 2105, 2700, 1269, 2551, 2660, 133, 3452]. **probed** [2095]. **Problem** [926, 1068, 870, 1073, 868, 845, 240, 3561, 1927, 3385, 1809, 1877, 1245, 2920, 3431, 2823, 557, 467, 2016, 2043, 2800, 2540, 2547, 581, 1748, 640, 323, 2477, 1196, 1316, 1190, 1377, 1660, 3712, 3363, 2481, 3692, 1336, 689, 26, 2174, 1006, 405, 214, 3190, 3191, 3192, 3430, 2079, 3251, 3488, 1940, 2676, 3150, 2638, 2637, 3156, 3125, 1848, 554, 3249, 1232, 3689, 3254, 2241, 3059, 3657, 2977, 2650, 2142]. **problem-solving** [3692, 3689]. **Problems** [842, 801, 806, 3400, 795, 863, 785, 2029, 2524, 2595, 2673, 2623, 2691, 2938, 2908, 3039, 2991, 1559, 3018, 329, 331, 409, 703, 2712, 2397, 612, 3493, 2828, 2364, 598, 2636, 3259, 3543, 3687, 2751, 2922, 3006, 3099, 3100, 2501, 2483, 2456, 3111, 1912, 2597, 2337, 3361, 3483, 3504, 3564, 2872, 3299, 3325, 383, 1038, 2927, 2943, 1710, 3662, 3012, 3596, 3005, 2064, 3113, 2346, 182, 1597, 2935, 2960, 3369, 3616, 3601, 3681, 3264, 3163, 3231, 3242, 3335, 3378, 3480, 3471, 566, 661, 3040, 3141, 3061, 2770, 3077, 3253, 2851, 2855, 3037, 3172, 3186, 3217, 3243, 3278, 3364, 3300]. **problems** [3152, 3268, 3280, 3349, 3302, 3316, 3497, 3586, 68, 77, 1399, 3269, 3508, 3332, 1382, 3147, 1525, 2213, 2057, 2818, 3235, 2954, 3063, 2284, 1386, 1781, 2558, 1677, 1684, 3101, 418, 2997, 2975, 3281, 3327, 3376, 3304, 3495, 3572, 3672, 3569, 2335, 2389, 3167, 3695, 3406, 3370, 3426, 3705, 322, 2574, 2868, 2971, 3160, 3187, 3218, 2648, 3044, 3592, 3724, 2699, 2994, 3064]. **Procedure** [928, 3493, 521, 1287, 1341, 2091, 566, 661, 3077, 95, 344, 3497, 2515, 2788, 2776, 590, 635, 2157, 3047, 3092, 3210, 203]. **Procedures** [756, 754, 3315, 666]. **proceeding** [2561]. **process** [1661, 1932, 2330, 2485, 3022, 467, 3130, 1602, 3365, 570, 71, 3089, 2388, 3377, 2694, 3403, 3073, 2869, 3617, 2353, 1925, 3297, 3138, 594, 700, 2413, 2512, 3236, 1625, 2616, 3656, 1306, 1358]. **processes** [974, 2412, 1676, 2596, 1686, 2502, 1780, 3350, 2359, 2044, 2955, 3681, 2091, 2541, 2499, 2725, 1724, 513, 405, 1212, 1386, 1781, 1234, 2822, 3279]. **processing** [2701, 2842, 3066, 3320, 3358, 187, 262, 2683]. **Procrustes** [2142]. **produced** [1769]. **produces** [1053]. **Product** [778, 2194, 685, 1865, 2996, 2388, 2250, 2318, 2423, 3261, 2262, 1606, 569, 644, 1739, 560, 622]. **production** [2316, 3022, 2121, 3668, 3640, 3675]. **Products** [827, 143, 1598, 1915, 3234, 422, 2493, 3072, 1929, 2833, 2882, 2293, 2332, 2707, 3290, 3219, 2512, 322, 615]. **Professor** [18, 2230]. **profile** [2502, 1198, 2766]. **profiles** [1824, 503]. **program** [665, 1094]. **programmed** [513]. **Programming** [1073, 1607, 456, 375, 1811, 1920, 2657]. **Progress** [3558]. **progressing** [2305]. **project** [1523, 1809]. **projected** [3182, 3708, 574, 125, 1790, 621]. **projection** [1744, 148, 1095, 288]. **projective** [1290, 1784]. **prolate** [1491]. **Proligand**

[1154, 1229, 2048, 2049, 2451]. **proligand-promolecule** [2048, 2049, 2451]. **proline** [2961]. **Promenading** [2898]. **promolecule** [2048, 2049, 2451]. **promolecules** [1229]. **Promoting** [249]. **Proof** [884, 883, 949, 957, 1632, 1735, 1860, 2573, 799, 74, 3549, 986, 679, 1298, 575, 653, 2076, 104]. **Propagating** [591, 2562]. **Propagation** [812, 824, 3184, 1891, 955, 2454, 344, 495, 436, 2327, 1403, 993, 1839, 2396]. **Propagator** [862, 73]. **propagators** [725]. **Propan** [1067]. **Propan-** [1067]. **Proper** [905, 1963, 2513, 1882]. **Properties** [1815, 1546, 1026, 756, 792, 803, 791, 2045, 2744, 201, 1071, 814, 878, 783, 578, 1059, 1100, 758, 1011, 769, 3338, 3647, 2938, 2991, 3686, 1236, 3721, 1795, 91, 168, 2367, 2137, 105, 261, 2879, 2587, 3390, 2103, 2534, 3318, 471, 2922, 1963, 3126, 15, 2815, 2688, 3652, 2535, 3374, 1545, 3655, 3325, 404, 227, 60, 2943, 147, 299, 3005, 1197, 2163, 3519, 1914, 2798, 2960, 279, 3175, 3221, 3264, 3231, 3335, 2856, 1895, 94, 2795, 2851, 2855, 3217, 3268, 3280, 3349, 3316, 1968, 1960, 3146, 317, 2850, 1635, 3147, 3394, 3423, 2157, 2546, 223, 51, 2844, 616]. **properties** [123, 3506, 3537, 3612, 636, 701, 277, 2133, 65, 2803, 2994, 2816, 3568, 1550, 3671, 3688, 2834, 1730, 3271, 326]. **property** [1064, 3004, 1395, 1533, 107, 2026, 3730, 3026, 979, 1464, 1463, 233, 1539, 3013, 1295, 1829]. **proposals** [1283]. **Proposed** [1967, 2130, 193, 2063]. **prospects** [1668]. **prostate** [1454, 2608]. **protease** [440]. **proteasome** [1763]. **Protein** [196, 341, 427, 1619, 1795, 291, 2477, 2961, 2543, 1702, 2415, 258, 590, 2013, 1267, 2279, 1847, 1913, 136, 3629, 3638, 1520, 2441, 2440, 3630]. **Proteins** [1089, 3161, 2234, 2031, 3629, 3638]. **proteomic** [2523]. **proteomics** [2080, 1864, 2279]. **Protochirons** [1449]. **protocol** [3647]. **protohelices** [1449]. **proton** [3320, 3358, 2861, 249]. **Protonation** [670]. **prototypal** [1809]. **prototype** [1787]. **pruning** [27, 85]. **pseudo** [1226, 2386, 1929, 251, 2332]. **pseudo-** [1226]. **pseudo-radioactive** [1929, 2332]. **pseudocentral** [1870]. **Pseudoharmonic** [1271, 1972, 3413, 3526, 1980]. **pseudorotation** [2028]. **pseudorotations** [2906]. **Pseudospectral** [1381, 3002, 1137, 3155, 1004]. **PT** [1019, 1156, 1247, 2290]. **PT-** [1019, 1156]. **PT-/non-PT-symmetric** [1019, 1156]. **PT-symmetric** [1247]. **published** [552]. **puckering** [1914]. **Pullen** [1328]. **Pulsating** [1818]. **pulse** [1515, 1584]. **pulsed** [1310, 1254, 1317, 1374, 1231, 1340]. **Pure** [3544, 2290, 1714, 1715, 3568]. **Putting** [1041]. **puzzles** [2458]. **pyridones** [194]. **pyrimidinyl** [1102]. **pyrolysis** [1202].

Q [1978, 3203, 3651]. **Q-rényi** [3651]. **QCT** [1296]. **QDM** [625, 624]. **QED** [2604]. **QM** [1534]. **QM/MM** [1534]. **QM/MM-ER** [1534]. **QMC** [2538]. **QMSI** [480]. **QMSM** [471, 480]. **QSAR** [714, 1418, 169, 1255, 1444, 266, 1587, 1801, 1380, 1440, 1430, 686, 1323, 3024, 2323, 1621, 1746]. **QShAR** [789]. **QSM** [1341]. **QSPR** [471, 744, 931, 2378, 2534, 2983, 3004, 3315, 3453, 3634, 977, 2555, 3631, 1255, 3626, 1106, 1372, 3458, 2607, 3047, 1565, 1551, 1601]. **QSPR-model** [1601].

QSPRs [2197]. **quadrangle** [2574]. **quadrangulation** [3263]. **Quadratic** [1022, 2402, 2271, 2254, 3000, 3174, 550, 3443, 1007, 1053, 2390, 2439, 436, 3197, 2192, 1573]. **quadratization** [3544]. **quadrature** [1451, 3440, 2040, 2718, 625, 624]. **quadratures** [2704]. **quadruplets** [2298, 2299, 2584, 2585]. **Quadrupling** [1072]. **quadrupole** [2362]. **Qualitative** [3410, 2168, 2079, 11, 2601, 4, 1647, 30, 31]. **Quality** [789, 500, 2323, 1739]. **quandles** [3161]. **Quantification** [2602, 1453, 2072, 2740, 2702, 2809, 2920, 3292, 3723]. **quantify** [2565, 2094, 3485]. **Quantifying** [3541, 383]. **quantisation** [1958]. **quantised** [2239]. **Quantitative** [2433, 1763, 2265, 2442, 3735, 471, 319, 128, 426, 427, 3460, 1647, 1539, 2133, 1314]. **Quantities** [915, 331, 3388, 583, 1766, 3659]. **quantization** [1963, 2513, 1882, 1481]. **Quantum** [890, 580, 384, 720, 3542, 816, 794, 942, 2202, 714, 866, 857, 928, 931, 930, 1052, 1070, 1066, 1885, 2058, 2443, 3453, 471, 1078, 2393, 3727, 1765, 799, 1852, 3541, 2382, 2345, 2527, 3425, 905, 3395, 2840, 245, 636, 701, 1784, 2671, 823, 2792, 3123, 3039, 472, 2514, 918, 244, 475, 3345, 974, 1971, 2412, 2453, 386, 2397, 2406, 3721, 3375, 483, 2672, 951, 467, 2367, 2986, 681, 2364, 491, 2082, 598, 597, 1369, 1370, 1341, 1598, 1989, 1953, 2106, 2153, 2383, 2540, 2547, 2534, 2649, 3323, 3634, 456, 480]. **quantum** [391, 3164, 2751, 3353, 2097, 1875, 500, 2160, 187, 2292, 2473, 3504, 425, 1946, 2408, 2533, 2715, 2872, 1241, 2186, 1321, 3089, 3012, 3005, 2727, 585, 256, 1758, 3264, 3242, 3335, 3378, 3471, 541, 3141, 3061, 1518, 2198, 3217, 3278, 3364, 3300, 3152, 3349, 3316, 3497, 3548, 1538, 3314, 1570, 2365, 2275, 2407, 2360, 2554, 3269, 1667, 2094, 3146, 3485, 3723, 2509, 2432, 3388, 2252, 3305, 3373, 3063, 2206, 596, 1872, 3569, 1335, 1410, 2704, 1407, 1414, 2338, 30, 31, 3058, 3426, 1076, 2396, 2458, 3491, 3160, 3187, 522, 560, 622, 577, 3069, 1278, 389, 390]. **quantum** [1835, 3134, 1044, 1054, 1253, 1446]. **quantum-chemical** [1835]. **Quantum-Mechanical** [799, 3542, 2514, 2364, 2408, 2533, 2715]. **quartet** [3431]. **Quartic** [3650, 475, 3664, 2738, 2439, 3304, 519]. **Quasi** [283, 2884, 2259, 1157, 1307, 811, 833, 2743, 492, 2330, 3224, 1926, 3344, 2777, 2181, 3048, 2011, 2427, 2066, 2139, 3381, 2251, 2767, 3588, 3151, 2214, 1721, 51, 48]. **Quasi-algebraic** [283]. **quasi-analytical** [2330]. **quasi-bi-Hamiltonian** [3588]. **Quasi-classical** [2743]. **quasi-degeneracy** [2214]. **quasi-linear** [3151]. **quasi-one-dimensional** [492]. **Quasi-Particle** [811]. **quasi-pentadiagonal** [3224]. **quasi-polynomial** [2767]. **quasi-polynomials** [2066]. **quasi-stationary** [48]. **Quasi-Steady** [833, 2884, 1926, 2011, 2427]. **Quasi-Steady-State** [2259, 3344, 2181, 3048, 51]. **Quasi-tree** [1157]. **quasi-tridiagonal** [2777, 3381]. **quasi-two-dimensional** [1721]. **quasichemical** [1213]. **quasiclassical** [255, 953]. **quasicrystal** [2790]. **quasicrystals** [2461, 2462, 2706]. **quasidegenerate** [527]. **quasirelativistic** [1385, 1475]. **quasitriangularity** [491]. **Quenching** [812, 824]. **queries** [1698]. **Questions** [927, 857, 1066, 801, 1948, 336]. **Quick** [3059]. **quinododimethides** [1492]. **quinoidal** [1976]. **quinolone** [194]. **quintet** [2180, 2183].

R [2785, 1209, 2452]. **R/S** [2452]. **R/S-stereodescriptors** [2452]. **Racah** [97, 1290]. **racemates** [2185]. **racemization** [194]. **Radial** [867, 889, 2595, 2673, 2623, 2691, 505, 362, 2283, 3674, 1747, 1465, 1466, 1350, 1456, 1599, 1600, 1764, 3080, 2349, 2605, 960, 2213, 967, 1099, 3150, 3545, 3552, 2704, 2380, 1993, 1407, 1414, 3452, 2594]. **radiation** [2071, 2343, 2327, 3669]. **radiation-damaged** [2343]. **Radiative** [1028, 2684, 1950, 2811, 1039, 1866]. **radical** [1040, 2041, 993]. **Radicality** [868]. **Radicals** [1188, 3536, 2562, 63, 621]. **radii** [3233, 3128, 1489]. **radioactive** [3590, 1929, 2332]. **radiobiological** [2905]. **radiotherapy** [2897]. **radius** [3291, 1506]. **rain** [2656]. **Raleigh** [3606]. **Raman** [3216]. **Ramani** [2395]. **Ramanujan** [1806]. **Randić** [702, 1176, 1220, 1121, 1265, 1002, 1088, 1347, 1031, 1157, 956, 1120, 1201, 1217, 1771]. **Randles** [895, 782]. **Random** [2242, 1413, 3286, 3700, 179, 1049, 2825, 2629, 152, 1005, 2384, 16, 153, 658, 3347, 2801, 1299, 3539, 378, 392, 2606, 2783, 1402]. **random-sampling** [1299]. **randomized** [3258]. **randomly** [197]. **Range** [922, 2832, 2101, 1050, 1205, 1284, 1447, 1595, 1659, 1769, 191, 1698, 1325, 406, 2116, 677, 192, 1907]. **ranges** [2732]. **ranging** [3184]. **Rank** [2310, 811, 395, 1153, 3045, 696, 89, 215, 733, 1478]. **Ranking** [977, 1361, 1255, 3093]. **rapid** [651, 983]. **rare** [250]. **rarefied** [674]. **Rate** [1061, 3582, 2316, 2344, 2249, 1808, 3000, 2873, 2152, 3303, 3122, 2355, 2193, 1296, 3662, 1283, 1842, 658, 3087, 2541, 2725, 1503, 1954, 1851, 378, 1704, 2819, 1276, 3423, 2194, 3707, 2428, 2839, 1772, 3271, 3492]. **rate-time** [658]. **Rates** [1152, 974, 1049, 3307, 2659, 3411, 3176, 3617, 1641, 1976, 1766, 1374]. **ratio** [3288, 2861, 530, 2864, 3425, 1145]. **Rational** [3474, 1451, 1843, 3285, 2535, 2659]. **rationality** [2277]. **ratios** [1571]. **Rauscher** [3731]. **ray** [2337, 1472, 3096]. **ray-based** [1472]. **Rayleigh** [3124, 728, 397, 564, 1804, 3708, 3691, 2242, 3355, 2159]. **Rb** [2376]. **RDA** [2437]. **re** [3634]. **re-constructing** [3634]. **reabsorption** [2404]. **Reachability** [1886, 1887, 1888, 662]. **Reactant** [2814, 2939, 3492]. **reactant-determined** [2939]. **reacting** [3599, 138, 2806]. **Reaction** [858, 1129, 2535, 937, 1152, 1134, 1047, 926, 450, 641, 1029, 802, 894, 824, 754, 3106, 3173, 3582, 2658, 3284, 2875, 1896, 3168, 3286, 2814, 974, 2316, 3713, 3247, 396, 2386, 2210, 3000, 3660, 3258, 1343, 3531, 1905, 2937, 3307, 135, 3103, 1472, 2845, 3731, 3303, 1740, 3589, 3122, 3711, 2998, 2502, 3514, 2884, 2659, 126, 1886, 1887, 1888, 1035, 1383, 1690, 1679, 2245, 1700, 953, 1296, 1260, 1605, 3699, 2388, 1842, 2359, 1834, 1920, 2096, 3363, 2019, 2913, 162, 2970, 2973, 3436, 658, 2910, 3087, 2955, 3034, 3726, 124, 2611, 410, 1568, 1626, 2215, 2105]. **reaction** [2228, 2177, 2199, 2313, 2419, 2454, 2559, 2628, 2615, 3140, 1292, 1836, 2219, 2505, 3110, 2244, 2583, 3008, 1861, 1319, 2281, 1718, 1464, 1463, 2293, 1693, 477, 495, 719, 2151, 2073, 2115, 1215, 1985, 2207, 2796, 2030, 514, 1851, 3246, 2776, 1641, 1976, 2676, 235, 3423, 2578, 1386, 1781, 1519, 2246, 3101, 3603, 2351, 2470, 3667, 699, 1848, 131, 1663, 738, 2921, 3467, 3584, 2641, 2924, 3153, 1974, 1434, 3406, 280, 731, 2536, 3249, 3611, 3704, 717, 715, 1485, 1616, 1825, 160, 1534, 2674, 3279, 1662, 682, 210, 1193, 3556, 591, 1625, 2881,

430, 484, 1997, 2065, 2577, 2422]. **reaction**
[2356, 2616, 3656, 2968, 3690, 3348, 3208, 2743, 3271, 2520].
reaction-convection-diffusion [3106]. **Reaction-diffusion**
[450, 2658, 2875, 2386, 3660, 3103, 1740, 2884, 2245, 2359, 2955, 3034, 2219, 2244, 2583, 3008, 1718, 1215, 2796, 3101, 2470, 3667, 2921, 3467, 3249, 591].
reaction-generated [3249]. **Reactions**
[777, 1107, 118, 903, 814, 757, 1061, 1084, 833, 3086, 3344, 19, 3287, 1291, 1362, 1277, 1808, 2636, 3226, 3660, 3451, 2643, 3294, 2355, 2494, 628, 3696, 2001, 605, 161, 2368, 674, 2045, 2927, 115, 2744, 1283, 364, 2014, 2974, 2140, 2141, 2094, 2819, 652, 524, 664, 2274, 2284, 1408, 3551, 988, 3619, 1911, 2348, 2467, 2561, 1248, 3518, 1819, 2574, 3556, 1789, 1786, 2487, 487].
reactions.Synthesis [972]. **Reactive** [1107, 255, 1734, 2474, 2774].
reactivity
[3303, 3451, 2457, 3620, 3581, 3591, 3534, 2094, 3485, 184, 494, 524, 2116, 2194].
Reactor [1020, 1013, 802, 894, 2964, 3658, 1931, 3386, 3436, 719, 3147, 699, 738, 1302, 1573, 2471, 2051, 1387]. **reactors** [1780, 1999]. **Read** [213, 212].
Reagent [845]. **reagents** [3307, 2512]. **Real** [862, 314, 313, 2338, 1137, 3114, 3501, 3258, 3698, 1814, 1698, 3730, 2675, 3693, 215]. **Real-Time** [862].
real-world [3693]. **realistic** [53, 54, 444]. **Reality** [2461, 2462].
Realizability [1025]. **Realization** [2264, 148, 3600]. **Realizations**
[2767, 1060, 3535, 2535, 2132, 2351, 1616, 1825]. **realm** [2898]. **rearranged**
[1907]. **Rearrangement** [1397, 396, 284, 3719]. **Rearrangements**
[1144, 1467, 259, 162]. **reasonably** [3504]. **reasoning** [1962]. **Reassessing**
[175]. **Recasting** [3000]. **receptor** [202, 3222]. **receptors** [590]. **reciprocal**
[386, 1576, 33, 452, 1342, 1589, 305]. **reciprocal-space** [386]. **Recognition**
[784, 1229, 63, 182]. **Recognized** [3735]. **Recognizing** [111, 211].
recombination [3536, 1760, 2882, 2512]. **Reconciling** [1770].
reconfiguration [710]. **reconstructed** [2920]. **Reconstructing** [1902].
Reconstruction [926, 3322, 997, 3431, 1545]. **Recoupling** [811, 944, 615].
recover [2238]. **rectangle** [2958]. **rectangles** [1403]. **Rectifying** [407].
recurrect [1542]. **Recurrence** [265, 1166, 473, 1329]. **Recursion**
[938, 1017, 936, 2888, 3678, 170]. **Recursive** [1530, 2537, 786, 3702].
recycling [1594, 3628]. **redefining** [3499]. **Redfield** [2237]. **Redheffer** [799].
REDIM [3330]. **Redlich** [3501]. **RedOx** [1880]. **reduce** [2900]. **Reduced**
[61, 789, 412, 1473, 413, 1908, 2189, 3500, 2990, 3429, 1660, 2917, 2752, 2232, 1788, 324, 2699, 1557, 326]. **reductase** [193, 1323]. **Reduction**
[884, 3066, 2777, 1881, 2075, 2884, 3072, 3610, 948, 2091, 1568, 1626, 2776, 2246, 3663, 3256]. **reductions** [2011, 2427, 697]. **Reductive** [2423]. **Rees**
[35]. **reference** [492, 33, 303, 2661, 1941]. **refined** [2791]. **Refinement**
[2782, 2480, 2339]. **Reflection** [1137, 2111]. **Reflections** [2182, 323, 2235].
reformulated [1730]. **regime** [2447]. **region** [1105, 3417, 2308, 2850, 1711].
Regions [3687, 1864]. **Regression**
[3395, 1362, 3446, 1749, 2025, 2548, 2700, 1801, 3403, 2399, 2883]. **Regular**
[1203, 1696, 1697, 263, 1164, 5, 1182, 544, 3263, 1495]. **regularity** [233].

Regularization [752, 3463, 3001, 1799]. **Regularized** [1299, 2591, 3446, 3732]. **Regulatory** [1011]. **reinforced** [3374]. **Related** [1126, 927, 1066, 786, 806, 863, 754, 2029, 2524, 2595, 2673, 2623, 2691, 1559, 1479, 638, 949, 957, 1258, 1632, 1735, 1860, 2074, 3053, 2828, 598, 2090, 207, 50, 645, 629, 991, 2358, 1690, 1679, 1664, 305, 1699, 13, 1597, 2228, 2177, 2199, 2313, 2559, 2628, 2615, 3140, 2505, 2062, 1704, 2213, 583, 205, 133, 1930, 2156, 2328, 1997, 2065, 2648, 2685]. **relatedness** [186]. **Relating** [923]. **Relation** [996, 3260, 887, 936, 2538, 2086, 3247, 2383, 1884, 2752, 7, 223]. **Relations** [3183, 3104, 914, 938, 1017, 1091, 770, 1166, 2366, 984, 3698, 217, 980, 999, 3678, 170, 1216, 693, 1441, 1667, 1719, 1364]. **Relationship** [3577, 780, 1316, 1190, 879, 922, 1757, 1763, 952, 2420, 1444, 2831, 603, 1325, 3723, 3623, 1539, 2133]. **Relationships** [1163, 1289, 924, 820, 831, 819, 761, 1496, 471, 3536, 319, 265, 2972, 3460, 233, 1329, 1610]. **Relative** [857, 987, 2712, 3043, 1194, 1303, 44, 183, 1732, 1724]. **relatively** [3497]. **Relativistic** [618, 3411, 3094, 3204, 3375, 3709, 1385, 1468, 1758, 1773, 1722, 1949, 2550, 730]. **Relativity** [2906]. **Relaxation** [1026, 795, 2224, 990, 996, 3294, 1553, 3373, 3101, 1977]. **relaxed** [2759]. **Relevance** [1085, 822, 1389, 668, 3554]. **Relevant** [850]. **reliability** [3194]. **reliable** [2248]. **remainder** [1777]. **Remark** [2559, 2628]. **Remarks** [326, 2589, 2434, 2615, 2033]. **removal** [3265, 1778, 1779]. **Renormalization** [2684, 2747, 2604]. **Rényi** [1982, 3273, 3311, 3729, 3574, 3416, 3425, 2123, 2350, 3651]. **Rényi's** [3437]. **Repair** [2344, 2254, 2343, 2905]. **Repeat** [882, 1126, 1258, 2074, 409, 1523, 1809, 1992]. **repeated** [1654]. **replication** [3237]. **Reply** [1027, 754]. **representability** [681, 2596]. **representable** [276]. **Representation** [496, 1092, 1141, 1075, 1797, 2397, 1655, 1578, 2827, 1369, 2540, 2547, 2858, 289, 2089, 2090, 231, 2833, 2035, 426, 427, 1299, 2184, 2700, 1207, 1180, 3403, 2126, 1852, 473, 2104, 958, 2038, 2423, 2707, 2791, 1259, 418, 73, 173, 988, 1988, 1947, 2204, 1739, 1879, 1810, 2050, 2459, 2460]. **Representations** [750, 910, 929, 1154, 766, 3339, 2837, 2309, 2653, 2981, 3085, 3710, 3694, 2012, 1900, 598, 1915, 2435, 3583, 1582, 3448, 109, 110, 161, 2907, 2936, 3145, 2243, 747, 2132, 647, 3715, 1295]. **Represented** [898, 2352]. **representing** [155, 1045]. **Repro** [815]. **Repro-Modelling** [815]. **Repulsion** [836, 2466, 2187, 563, 2600]. **repurposing** [3642]. **requires** [3551]. **research** [3346]. **residence** [1780, 2046]. **residual** [3136, 2883]. **Resistance** [1353, 290, 781, 3555, 1731, 1502]. **resistance-distance** [1502]. **resistances** [2620, 3166]. **Resolution** [2255, 3385, 949, 957, 1632, 1735, 1860, 2185, 1454, 2072, 3066, 3288, 3292, 3538, 3604, 3570, 3720, 693, 1354, 1235, 1476, 1641, 1976, 1788, 440, 3013]. **resolved** [3500]. **Resolving** [3657]. **Resonance** [1085, 792, 1390, 2134, 1169, 16, 892, 1139, 1389, 1453, 1443, 1901, 2072, 2255, 2431, 2608, 2651, 2580, 2602, 2741, 2794, 2773, 2702, 3066, 2967, 3320, 3358, 2863, 2122, 2374, 1012, 1726, 616, 2926, 1919]. **Resonances**

[3206, 2701, 3205, 3697, 2715, 1642]. **Resonant**
[3614, 843, 1221, 1000, 1345, 2697, 2853]. **resource** [2292, 1583]. **resources**
[2409]. **Respect**
[1172, 1236, 1176, 3148, 434, 1553, 3041, 1575, 1500, 1845, 998]. **respectively**
[3581, 3534]. **respirometers** [1204]. **Response**
[901, 838, 1789, 2741, 2367, 2165, 3324, 488, 1316, 1190, 1515, 3643, 1553,
3332, 1204, 3675, 533, 950, 1386, 1340, 1301, 2610]. **responses** [1302, 1387].
Restricted [796, 2757, 2311, 2824, 315, 572]. **restriction** [3392].
Restrictions [2367, 2100]. **restrictive** [2088, 2100]. **Restructuring**
[850, 904, 820]. **result** [603]. **Resultant** [2497, 2667]. **resulting** [3210].
Results [764, 1142, 2669, 1546, 681, 501, 502, 523, 177, 2801, 1242, 1574,
3341, 3029, 3473, 2962, 2338, 3619, 634, 1854]. **retention** [3622]. **Retro**
[1423]. **Retro-Leapfrog** [1423]. **Returnability** [2001]. **returning** [264].
reveal [2238]. **revealed** [3076]. **revealing** [231, 3514]. **Reversal**
[3035, 1467, 1196]. **Reversals** [1144]. **reverse** [3627, 1593, 1589].
reversibility [1920, 1648, 2454, 1990]. **reversible**
[1896, 3535, 709, 3342, 2973, 2259, 2925, 2351, 230, 3707, 3690]. **reversion**
[2155]. **Review** [1669, 1668, 2967, 759, 923, 552, 3646, 142, 56, 3341].
reviews [680]. **revised** [2028, 2358, 3422]. **Revisited** [877, 3120, 2150, 3585,
3329, 3402, 1636, 2953, 566, 661, 1898, 2033, 2400, 1232, 2520]. **revisiting**
[2755]. **Revival** [2630, 3343, 2703]. **Rg** [1096]. **RGA** [3658]. **rheometer**
[2874]. **Rhombellane** [2969]. **rhomboidal** [3475]. **ribbon** [258, 288].
Riccati [1021]. **rich** [1675]. **Richardson** [3202, 3310]. **Ridge** [2154, 2041].
Riemann [3481, 3208]. **Riemann-Zeta** [3481]. **Riemannian** [3432, 1346].
Riga [3590]. **Rigby** [1521]. **Right** [767, 611, 371, 553]. **rigid**
[2705, 2653, 1130, 2465, 3451, 468, 2862, 546, 1944, 1844, 469, 739].
rigid-rotor [1944]. **Rigorous** [1889]. **Ring**
[259, 816, 954, 2986, 523, 3514, 2041, 433, 1742, 2078]. **ring-opening** [3514].
ring-shaped [954, 1742, 2078]. **Ring-transformation** [259]. **Rings**
[893, 933, 3721, 978, 360, 1804, 224, 1914, 956]. **rippled** [2164]. **Ritz**
[3606, 3708, 3691, 3355]. **rivality** [3024, 3194]. **river** [2525]. **RKN** [2110].
RNA [1279, 3071, 510, 1207, 1180, 1075]. **Ro** [1514, 2352]. **Ro-vibrating**
[1514]. **Ro-vibrational** [2352]. **Roadmap** [2201]. **roaming** [2910]. **Robin**
[3483]. **Robinson** [2931]. **Robust**
[2794, 3677, 367, 2494, 3034, 2515, 3595, 3467, 1756]. **rocks** [2225]. **Rod**
[767, 3357, 2705, 611, 1450, 553, 672]. **Rod-Like** [767, 611, 553, 672].
Rod-packing [3357]. **Rodriguez** [3245]. **rods** [197]. **Role**
[865, 2984, 1139, 1545, 2187, 407, 2621, 33, 1622, 662, 1976, 615]. **Root**
[827, 2647, 3372, 3439, 231, 201, 3407]. **root-finding** [3372]. **rooted** [3261].
Roothaan [1366, 1471, 1595]. **roots** [2901, 2952, 3602, 3259, 2482, 2891].
Rosen [1052, 3164, 1124, 1963, 1882, 608, 2227, 3289, 3002]. **Rota** [277].
rotating [3329, 3566, 20, 3663]. **rotation**
[204, 1814, 1477, 563, 485, 613, 1350, 1456, 2661, 1329, 1511, 1670].
rotation-angular [1814, 1350, 1456]. **rotation-vibration** [1477]. **rotational**

[3051, 538, 2360]. **rotator** [491, 2465]. **rotaxanes** [312]. **rotor** [468, 1944]. **rotors** [3195]. **Rough** [880]. **round** [1918]. **route** [1612]. **row** [3709]. **RS** [1299, 3456, 3457, 3468, 2027, 2028, 2298, 2299, 2371, 2372, 2450, 2451, 2452, 2584, 2585]. **RS-HDMR** [1299]. **RS-stereogenic** [2452]. **RS-stereogenicity** [2451, 2027, 2028]. **RS-stereogenicity/RS-stereoisomerism** [2028]. **RS-stereoisomeric** [2450, 3456, 3457, 3468]. **RS-stereoisomerism** [2028]. **RS-stereoisomers** [2299, 2371, 2372, 2584, 2298, 2585]. **Ru** [1170]. **Rubber** [2874, 579, 2711, 3001]. **rule** [130, 1486, 1279, 291, 1963, 2513, 1481, 127]. **Rules** [439, 464, 490, 1353, 1882, 345, 3551]. **Runge** [2178, 2322, 966, 1114, 1559, 2283, 2893, 3674, 2943, 3610, 806, 1597, 2143, 2334, 3026, 3061, 2024, 2507, 607, 771, 1541, 2914, 2699, 2835]. **Rushbrooke** [209, 103, 285]. **Rychlý** [894]. **Rydberg** [992, 1118, 1325, 1820, 35].

S [2872, 1483, 953, 1296, 1260, 552, 1435, 2968, 3424, 2030]. **S-stereodescriptors** [2452]. **s10910-008-9398-z** [1483]. **Sacker** [3455]. **Sagar** [2785]. **salinity** [2571]. **Sal'nikov** [372]. **Same** [933, 2127, 2126]. **Samples** [766, 3124, 3431, 1925]. **sampling** [1929, 1299]. **Sanderson** [970, 1069]. **Santamaria** [1869]. **Saturated** [853, 2191, 626]. **Saturation** [1257, 3690]. **sausage** [3733]. **Saxon** [1280]. **Saxton** [3440]. **say** [1926]. **SBVPs** [3266]. **SC-EHT** [2463]. **scaffold** [2026]. **scaffold-based** [2026]. **Scalability** [1082]. **scalable** [1927, 2026]. **Scalar** [827, 677, 1598, 1915, 3234, 1464, 1463]. **Scale** [772, 1089, 287, 2742, 1568, 1626, 2038, 2315, 3068]. **Scaled** [1952, 875, 1004]. **scales** [341, 1731]. **Scaling** [860, 1895, 2031, 3392, 2843, 1736, 427, 1847, 1913, 961]. **scandium** [2424]. **scanner** [3570]. **scatterers** [677]. **scattering** [708, 255, 2951, 675, 2379, 1269, 554, 732]. **scavenger** [993]. **SCF** [2148, 720]. **Scheme** [886, 3106, 415, 2901, 3575, 3404, 275, 1881, 3012, 3712, 3005, 2935, 2960, 3601, 3653, 3159, 3110, 2974, 3186, 3243, 3547, 2229, 3327, 3509, 3603, 3391, 682, 3546, 3044, 3510, 3064, 3310]. **schemes** [1971, 2412, 2760, 3483, 1540, 556, 3707, 2880, 3014, 3732]. **Schmidt** [2748, 2749]. **Schnakenberg** [2437, 3157, 2219, 3454]. **Schottky** [2686]. **Schrödinger** [3639, 2034, 954, 1224, 1870, 3129, 728, 1745, 1754, 1798, 1871, 2060, 2029, 1956, 2118, 2178, 2253, 2410, 2322, 2544, 2524, 2549, 2472, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 966, 1114, 1559, 1479, 1527, 1526, 1486, 1972, 684, 763, 764, 817, 2764, 2734, 2746, 2828, 397, 564, 743, 984, 1804, 625, 2468, 3487, 2110, 2283, 2893, 3674, 3313, 1021, 2035, 2566, 1247, 806, 965, 1633, 1695, 1840, 1597, 2633, 3159, 2143, 2334, 3026, 1381, 840, 841, 2733, 3088, 2349, 2554, 2336, 964, 1098, 1174, 2024, 3002, 2507, 3295, 3276, 3354, 2511, 2639, 1980, 2213, 967]. **Schrödinger** [1099, 1678, 968, 2211, 1266, 1271, 2380, 3199, 607, 637, 713, 771, 800, 863, 912, 1101, 1357, 1355, 1548, 1904, 1993, 2098, 1407, 1414, 2338, 2930, 2590, 188, 1396, 837, 1165, 1294, 2007, 832, 963, 1528, 1549, 2720, 3033,

2648, 2522, 2775, 2835, 3030, 3732, 1614, 2078, 2697, 2853, 2719, 2594]. **Schur** [615]. **Schwarz** [3101]. **Schwarzite** [2915, 2916]. **Science** [3015, 1930]. **Sciences** [959, 2568]. **scientific** [1615, 2111]. **scorch** [1717]. **Scott** [3552]. **Screened** [919, 1132, 1156, 1133]. **Screening** [1079, 1127]. **screw** [2046]. **Se** [2376]. **Search** [1175, 2845, 962, 3067, 345, 317, 218]. **searching** [280]. **seasonally** [1254]. **Secant** [2894]. **Secant-like** [2894]. **Second** [3404, 121, 3355, 2903, 1174, 1177, 1201, 1754, 2029, 2178, 2410, 2322, 2544, 2524, 2549, 2472, 2623, 2662, 2691, 2709, 2938, 2908, 2991, 1523, 1809, 2367, 470, 2922, 1912, 3564, 60, 2943, 3712, 1994, 547, 2935, 2960, 1648, 2541, 2499, 2725, 3378, 3528, 2770, 2717, 3450, 2733, 2795, 2851, 2855, 2221, 2867, 3508, 2507, 2511, 571, 2036, 3595, 3569, 2317, 2455, 2475, 3693, 3058, 3370, 1500, 1845, 682, 3556, 1264, 2971, 2302, 2648, 2994, 2931, 2594]. **Second-order** [3404, 121, 1174, 470, 60, 3712, 547, 3528, 2867, 2036, 3595, 3569, 2475, 3693, 682]. **Secondary** [1951, 1075, 1279, 196, 341, 1207, 1180]. **section** [3576, 1260, 2296]. **sections** [3132, 3685, 3424]. **sedimentary** [2225]. **Seeing** [46]. **selected** [2225, 1194, 1303]. **selecting** [3046, 2331]. **selection** [744, 3294, 3446, 3628]. **Selective** [1055, 367, 3158]. **selectivity** [2167, 461]. **Self** [768, 1105, 1038, 1743, 243, 1406, 2303, 242, 2536, 2525, 1161, 2463, 3066, 746, 2421, 2862, 2714, 2742, 669, 264, 1450, 2289, 635, 3473, 3237, 2838, 3380, 1638]. **self-assembling** [669]. **self-assembly** [2862]. **Self-avoiding** [1406]. **Self-consistent** [1105, 243, 242, 1161, 2463]. **self-consistent-field** [2742, 635]. **self-correcting** [3066]. **self-energies** [2421]. **self-intersections** [1450]. **Self-Parametrization** [768]. **self-replication** [3237]. **self-returning** [264]. **Self-similar** [1038, 1743, 2525, 2714, 2838, 3380, 1638]. **self-similarity** [746]. **Self-sustaining** [2536]. **Selfadjoint** [1984, 2231, 2745]. **Selfcomplementary** [2257]. **selfreverse** [2257]. **Sel'kov** [3454, 1703]. **Semi** [3178, 3447, 2318, 2658, 3542, 3673, 3353, 2213]. **semi-analytical** [2658]. **Semi-Cartesian** [2318]. **semi-classical** [3542]. **semi-embedded** [2213]. **Semi-exact** [3178, 3447]. **semi-implicit** [3673]. **semicircle** [2504]. **Semiclassical** [3414, 1988]. **Semiconductor** [1078, 1378, 2206]. **semiconductor-metal** [2206]. **semiempirical** [483]. **semiexplicit** [1535]. **Semigroup** [2666]. **semigroups** [2523]. **SEMILAM** [1306]. **semilocal** [2895]. **semiregular** [1654]. **Semispaces** [927, 827, 1370, 1915, 2984]. **seniority** [2865]. **Sense** [1056]. **sensitivities** [1653]. **Sensitivity** [2485, 2480, 116, 1849, 3576, 457, 2752, 2776, 3209, 1691, 48, 2839, 64, 65]. **sensors** [1208]. **separability** [2320, 1365]. **separabiliy** [3216]. **separable** [1613, 1837, 2007]. **separate** [1306]. **separated** [1788]. **Separation** [886, 2226, 1922, 1443, 2272, 3301, 726, 1306]. **septic** [3397]. **Septupling** [1072]. **sequence** [438, 278, 1267, 1563]. **Sequences** [1092, 1141, 1135, 1578, 1900, 3076, 1846, 1219, 1702, 1716, 2257, 2523, 2273, 1295, 1273, 1339, 2821, 1557]. **Sequential** [833, 179, 456, 3067]. **Series** [923, 3582, 2514, 2538, 475, 36, 2397, 2952, 2861, 2827, 1805, 1793, 2878, 14, 3553, 2319, 2320, 3057, 2042, 2077, 3084, 3462, 1826, 1983, 2117, 2335, 3249,

519, 2799, 1638]. **Set** [1016, 1208, 1661, 3385, 496, 2058, 2103, 3583, 275, 3296, 3606, 183, 1398, 2008, 3290, 1721, 2260, 2640, 433, 440]. **Sets** [1014, 1056, 811, 1148, 568, 598, 597, 1989, 1953, 2136, 3071, 3486, 995, 1701, 1095, 227, 1205, 1321, 1284, 1338, 1385, 1468, 1475, 1604, 2682, 93, 1884, 1852, 692, 2707, 571, 2305, 536, 1290, 3625, 2323, 459, 696, 697, 2023, 3600, 2805, 711]. **Sevcik** [895, 782]. **Seven** [2238]. **seventh** [2892, 1099]. **seventh-order** [2892]. **several** [1807, 408, 3111, 513, 522, 1044, 1054]. **sextet** [227, 3221, 104, 2084, 1650]. **sextets** [15, 998]. **sextic** [3178, 3313, 3447, 3295]. **sextuple** [284, 2650]. **Shadow** [3315]. **Sham** [2426, 3547]. **Shannon** [3120, 3389, 3490, 3479, 3727, 3476, 1774, 1899]. **Shannon-like** [1774]. **Shape** [52, 1280, 927, 43, 693, 327, 1675, 897, 1378, 3470, 1970, 253, 287, 2842, 2809, 3292, 3500, 3735, 2103, 2131, 434, 426, 427, 2565, 156, 315, 307, 692, 1440, 1968, 1918, 1432, 1969, 2528, 599]. **Shape-invariance** [1280]. **Shape-similarity** [693]. **shaped** [954, 41, 1742, 2078, 3492]. **Shapes** [790, 791, 46, 44, 183, 1918]. **shared** [985]. **Sharp** [1262, 1177, 3699]. **Sheet** [861, 2624]. **Shell** [1151, 846, 2755, 598, 1973, 3155, 1595, 1327, 2324, 572, 1455, 1534, 827]. **Shells** [1915, 1665, 1366, 228]. **Sherman** [1312, 1748, 3149]. **shielding** [1722]. **Shift** [1046, 400, 1989, 3583, 515, 26, 554]. **shifted** [2099, 3025]. **shifting** [2103, 2257]. **shifts** [2176, 134, 2926]. **Shishkin** [3565, 3397]. **shooting** [2016, 2043, 2384]. **Short** [3206, 3205, 2101, 3303, 1239]. **short-range** [2101]. **short-term** [3303]. **Should** [1396]. **shrinking** [2693]. **Shrödinger** [867, 889]. **Shtrikman** [2479]. **Shull** [2087]. **Si** [1685, 1545, 173, 1544, 1547]. **side** [623, 30, 2769]. **sided** [1113]. **sigma** [202]. **sigmoid** [447]. **Sign** [1605]. **Signal** [3358, 1443, 2701, 3066, 3288, 3320, 1307]. **signal-noise** [1443]. **signal-to-noise-ratio** [3288]. **Signals** [3206, 61, 1389, 1453, 2431, 2741, 2740, 2842, 3083, 3205, 3500, 3538, 3570, 3697]. **signature** [3048]. **Signatures** [857]. **Significance** [940, 3669, 60, 3625]. **significant** [22, 157]. **Signs** [857]. **SiH** [2093]. **silica** [1897, 2433, 1981]. **silica-supported** [1981]. **silicate** [2663, 2871]. **silico** [2902, 3629, 3638]. **Silicon** [1617, 1546, 1544]. **silicon-germanium** [1544]. **silver** [3659]. **Similar** [945, 1038, 1743, 2714, 2838, 3380, 2525, 1638]. **similarities** [551]. **Similarity** [1206, 1070, 1066, 1079, 93, 474, 1219, 1141, 809, 3478, 257, 3541, 897, 494, 524, 580, 1757, 746, 1324, 1900, 520, 597, 714, 1369, 1370, 1341, 1598, 1885, 2058, 1953, 1915, 2106, 2109, 2540, 2547, 2443, 3323, 3453, 3634, 471, 480, 3164, 529, 335, 3311, 3651, 1095, 3627, 3445, 32, 56, 1852, 1041, 43, 156, 693, 1667, 2094, 3146, 3485, 3723, 1445, 3425, 2677, 596, 1323, 3703, 1899, 2323, 2528, 3452, 1273]. **Simmons** [1223, 2949, 1575, 1186, 1264, 1230, 1109]. **Simple** [1142, 2131, 1138, 686, 2574, 833, 1615, 2614, 3396, 283, 3365, 2077, 1717, 378, 2144, 2214, 2031, 616, 3154, 2133, 487]. **simplest** [658, 1503, 1954]. **simplex** [2607]. **simplex-informational** [2607]. **simplexes** [327]. **simplified** [3712, 2236, 1866]. **Simulate** [874, 3055]. **simulated** [2290, 2393, 2439, 561]. **Simulation** [707, 861, 3711, 1032, 774, 3070, 3647, 1680, 2705, 2875, 1880, 1955, 2095, 2210, 3517, 3330, 3676, 1671, 2947, 1003,

2044, 2955, 1425, 3539, 2694, 2897, 1100, 3552, 3102, 1436, 1409, 3688]. **simulations** [1971, 2510, 2624, 3383, 455, 3035, 530, 2946, 2405, 3568]. **simultaneous** [3288, 2210, 2502, 1853, 3675, 1550]. **sine** [3056, 3645, 2184, 3042]. **sine-discrete** [2184]. **sine-Gordon** [3645, 3042]. **Sinelshchikov** [3150]. **Single** [2181, 1946, 814, 878, 873, 833, 825, 2070, 472, 1896, 1777, 1094, 2249, 3489, 3535, 2121, 2898, 2899, 1194, 1303, 2863, 2306, 2819, 2046, 3550, 1583, 1981, 2787, 1253, 2900]. **Single-Molecule** [878]. **single-particle** [1981]. **single-screw** [2046]. **single-species** [1583]. **Single-substrate** [2181, 2819]. **single-walled** [2070]. **singlet** [3697]. **singlet-appearing** [3697]. **singly** [3165]. **singly-bordered** [3165]. **Singular** [752, 1068, 2471, 2231, 1984, 3375, 3687, 3483, 3616, 2668, 2113, 3430, 2558, 2638, 2637, 2997, 3281, 3327, 3376, 3304, 3572, 3672, 2618, 3693]. **singularities** [949, 957, 1632, 1735, 1860, 2161, 2899, 644]. **singularity** [36, 3682, 3705, 2577]. **Singularly** [3400, 3106, 3565, 3361, 3325, 3712, 3594, 2064, 3363, 3034, 3397, 3725, 3681, 3378, 3480, 3471, 3364, 3300, 3302, 3316, 1677, 1684, 3101, 3595, 3197, 3199, 3391, 3467, 3695, 3370, 3426, 2241]. **sintering** [2055]. **sinusoidal** [1906]. **SIR** [3247]. **site** [169, 2882]. **site-specific** [2882]. **sites** [2976, 2127, 2126, 2306]. **situated** [1890]. **Sivashinsky** [3706, 3559]. **six** [2392, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 2938, 2908, 3116, 2764, 2734, 2746, 2733, 2851, 2855, 3186, 3199, 1806, 2381, 3081]. **six-step** [2392, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 2938, 2908, 2764, 2734, 2746, 2733, 2851, 2855, 3199, 2381, 3081]. **sixteenth** [3372]. **sixteenth-order** [3372]. **Sixth** [967, 2908, 2904, 2903, 3125]. **sixth-order** [2904]. **Size** [1913, 3396, 434, 3456, 3035, 1192, 2788, 712, 3435, 1847, 2031, 1806, 1941, 413]. **size-consistency** [413]. **size-extensive** [1941]. **Sizes** [2771, 2053, 7]. **Skeletal** [2917, 424, 3074]. **skeleton** [1461, 1462]. **skeletons** [2862, 3145, 4]. **skew** [2136]. **slabs** [1406]. **Slater** [920, 1483, 1600, 1027, 2287, 3202, 836, 917, 919, 971, 1017, 1321, 1379, 1246, 1385, 1468, 1471, 1447, 1595, 1604, 1350, 1456, 1599, 1482, 854, 946, 1459, 1460, 1261, 401, 1907, 356]. **Slater-type** [1907]. **Sliding** [776]. **slits** [1406]. **Slow** [3640, 2474, 3373, 11, 2774]. **slower** [3492]. **Small** [2514, 287, 414, 846, 3106, 1543, 1545, 2242, 747, 1441, 1918, 2038, 3197]. **Small-** [287]. **Small-energy** [2514]. **Smallest** [430, 1227, 1974, 484]. **Smeared** [3232]. **SMILES** [1621]. **SMILES-based** [1621]. **Smith** [3583, 1521]. **Smoluchowski** [3698, 2470]. **Smoluchowski-type** [3698]. **Smooth** [1351, 3582, 2658]. **SNR** [3720]. **SNR-resolution** [3720]. **SNS** [1443]. **Soai** [2568]. **Soai-autocatalysis** [2568]. **Sobolev** [720, 743]. **sodium** [1827]. **soft** [2203, 2466, 3308]. **softness** [3620, 3581, 3591, 3534, 3723]. **software** [2018, 2369, 1707, 2091]. **Soil** [272]. **soils** [3434]. **solar** [2687]. **solenoidal** [3357]. **Solid** [658, 1160, 461, 3710, 1291, 1362, 1277, 972, 2044, 3368, 3367, 558, 1409, 1376, 2366]. **solid-state** [1291, 1362, 1277]. **solids** [918, 1042, 3210]. **solitary** [2582]. **Soliton** [2232, 2395]. **solitons** [3091]. **solubility** [1565]. **Soluble** [835, 534, 689]. **solute** [1807, 1794]. **Solution**

[890, 1114, 763, 764, 3504, 806, 855, 2419, 3497, 1174, 3394, 771, 800, 863, 912, 3426, 3611, 867, 889, 832, 1614, 89, 954, 3129, 1745, 1871, 2029, 1956, 2118, 2178, 2524, 2549, 2673, 2623, 2662, 2691, 2709, 1666, 966, 1559, 1479, 1527, 1526, 2553, 3722, 684, 1676, 2330, 3086, 2343, 1655, 2764, 2734, 2746, 1494, 3565, 400, 2802, 625, 2418, 3155, 1878, 273, 445, 2468, 1312, 1987, 3676, 3122, 2110, 2183, 2319, 2320, 2695, 3544, 1552, 3057, 1097, 1477, 2297, 965, 3650, 2064, 3170, 1633, 1695, 1597, 3725, 3653, 2611, 3262, 2149, 624, 3308, 1045, 1336, 2143]. **solution** [2334, 2847, 3026, 1381, 1861, 3513, 2851, 2554, 2489, 3459, 3559, 405, 3002, 2507, 2511, 2529, 2213, 1036, 2484, 2119, 967, 1099, 1519, 1677, 1684, 968, 2758, 2211, 1266, 1271, 3239, 2380, 3199, 1234, 607, 637, 713, 1101, 1548, 1904, 2098, 1407, 1414, 2033, 2335, 3584, 2092, 2413, 2978, 1238, 519, 2830, 3398, 963, 2236, 517, 2720, 3211, 2648, 3042, 1644, 2719, 2594, 2792]. **Solutions** [1696, 1697, 3466, 1019, 2035, 1171, 3355, 2941, 840, 841, 2336, 3074, 2675, 881, 1165, 3639, 2034, 2658, 2938, 2908, 3385, 2032, 1972, 2010, 3054, 3648, 1315, 2498, 3247, 3413, 1401, 595, 2386, 743, 2571, 416, 3393, 3096, 3536, 3056, 3178, 3487, 2492, 645, 1156, 3299, 3447, 3020, 736, 3215, 3699, 3386, 2480, 2014, 2541, 2499, 2725, 1292, 3714, 3679, 2896, 3227, 449, 3008, 2855, 1693, 2349, 1215, 2713, 3524, 3198, 3332, 3354, 2639, 3147, 1980, 2145, 1329, 1525, 652, 3290, 3235, 3423, 2232, 2333, 3545, 3136, 601, 3237, 2347, 1434, 3406, 1977, 2590, 3333, 3518, 1396]. **solutions** [3272, 3707, 2963, 3236, 3615, 2574, 2525, 2135, 2395, 1772, 1742]. **Solvability** [2556]. **Solvable** [2291, 1224, 2082, 1181, 657, 1837, 2840]. **solvation** [2755, 595]. **solve** [557, 3313, 656, 3369, 3295, 3359]. **solved** [2920, 1963, 1882]. **Solvent** [245, 244, 3184, 402]. **solvents** [1565]. **solver** [2158, 3114]. **Solving** [3561, 2553, 2644, 2456, 3483, 2184, 3400, 3276, 2284, 3249, 1084, 845, 3106, 1797, 3023, 3018, 3224, 3099, 3100, 3439, 2483, 2760, 3111, 1472, 3564, 2283, 3674, 3312, 2477, 2927, 1751, 3662, 3596, 1741, 2139, 3593, 3645, 3516, 3440, 3363, 2481, 3702, 3471, 3692, 2974, 2894, 2903, 3548, 3244, 2057, 3150, 2638, 2637, 2997, 2975, 3156, 3125, 3281, 3327, 3376, 3603, 3572, 3569, 2389, 2475, 3167, 3274, 3689, 2868, 3081, 2626, 2302, 2723, 3724, 1322, 1816, 2501]. **Sombor** [3683, 3238, 3341]. **Some** [3123, 2589, 1142, 1128, 2434, 501, 502, 523, 794, 1162, 1163, 857, 801, 3111, 177, 803, 1986, 589, 182, 336, 1143, 2615, 1110, 1574, 3029, 1399, 3049, 3246, 3473, 2546, 1060, 607, 123, 555, 899, 1730, 685, 3129, 3031, 639, 2879, 3104, 2111, 3632, 181, 3631, 352, 2513, 3299, 2870, 3143, 1753, 3553, 3666, 1751, 1363, 986, 1994, 1164, 28, 357, 1801, 3513, 1895, 2776, 1980, 2057, 3235, 3359, 3537, 3707, 277, 322, 2958, 1816, 2487, 65]. **Somehow** [2899]. **Sommerfeld** [1958, 2827]. **sophisticated** [3608]. **sorbed** [3007]. **Sorbie** [1308]. **sorption** [2398, 272, 1733, 2830]. **sound** [2940, 3058, 2912]. **source** [3106, 1799, 1925, 2157]. **sources** [1933, 2158, 2391]. **Space** [330, 882, 1126, 778, 916, 2111, 791, 1187, 2900, 902, 1059, 2526, 580, 1696, 1697, 3051, 1982, 2895, 409, 1258, 1523, 1809, 1992, 2074, 2453, 386, 1892, 479, 3009, 3680, 408, 1893, 2112, 2383, 442, 443, 2161, 2969, 1252, 2075, 3137, 1388, 2320, 2888, 3347, 2910, 3087, 1698, 279, 183, 315,

327, 3416, 1776, 2205, 2405, 2979, 1408, 1100, 3552, 1407, 1414, 2338, 3405, 2192, 602, 277, 459, 67, 3414, 2805, 1293, 326, 463, 356, 545, 1252]. **space-time** [3405]. **Spaces** [914, 2731, 811, 1523, 1809, 2837, 720, 598, 743, 984, 1346, 2153, 2125, 2665, 2782, 3071, 2982, 3255, 3275, 3277, 3234, 3318, 3315, 3453, 3634, 391, 3164, 1095, 1205, 1284, 1338, 1385, 1468, 1604, 56, 979, 3107, 2551, 2527, 737, 1774, 696, 697, 413]. **Spain** [3015]. **Spanned** [1187]. **spanning** [429, 2933, 388, 2377, 98]. **Sparse** [2548, 2399, 3045, 1616]. **Spatial** [2808, 318, 342, 3725]. **Spatial-fractional** [2808]. **spatially** [2116, 2194]. **Spatiotemporal** [3298]. **speak** [3557]. **Special** [2886, 884, 2837, 3360, 3621, 357, 1282, 1850, 959, 3511, 1233, 3097]. **specialised** [2777]. **Species** [834, 3385, 3599, 3589, 2369, 1887, 1660, 1365, 1583, 1823]. **Specific** [525, 2173, 3381, 2882, 2621, 2788, 607, 3058, 1819, 2883]. **Specification** [493]. **specified** [346]. **Spectra** [851, 1188, 907, 2612, 3686, 3710, 3737, 3736, 1454, 2701, 2740, 2842, 2920, 3604, 3570, 3697, 2137, 1351, 1395, 2464, 3661, 559, 631, 1306]. **Spectral** [3736, 3201, 858, 3175, 3547, 3291, 330, 3484, 3481, 3734, 1305, 1578, 2161, 2748, 1533, 3216, 2216, 1506, 1647, 2558, 3274, 1004, 2749, 1489, 3737]. **spectral-based** [3481]. **Spectroscopic** [2513, 2431, 2608, 2602, 2794, 3446, 1844, 3659]. **spectroscopies** [3475]. **Spectroscopy** [3339, 1085, 3206, 472, 1139, 1389, 1453, 1443, 1901, 2071, 2072, 2255, 2651, 2580, 2741, 2773, 2702, 3066, 2967, 3205, 3288, 3292, 3320, 3358, 3500, 3538, 3604, 1324, 435, 248, 2352, 192]. **spectrum** [918, 1963, 87, 1882, 3109, 2377, 960, 958, 3263, 2703, 2745, 1620]. **speed** [3730, 3058, 2912]. **speeds** [2940]. **SPH** [1687]. **sphere** [1744, 149, 3451]. **spheres** [197, 3255, 2722]. **Spherical** [3499, 1166, 773, 395, 2964, 366, 2519, 3374, 1986, 2042, 1477, 3319, 1996, 1895, 2565, 3354, 3469, 3290, 2206, 2921, 3717, 3211, 3628, 1866]. **spherically** [2665, 2429]. **Sphericities** [1154]. **Spherocylindrical** [767, 611, 553]. **spiked** [2429]. **Spillover** [2348]. **Spin** [816, 796, 2385, 412, 2130, 2341, 2906, 746, 400, 501, 502, 523, 2996, 3479, 574, 1338, 3547, 2140, 3541, 3191, 1290, 1949, 2550, 277, 322, 459, 525, 555, 614, 2441, 2440]. **spin-** [400]. **Spin-adapted** [412]. **spin-boson** [2140]. **spin-coupling** [2441, 2440]. **spin-density** [3547]. **spin-nonadapted** [412]. **spin-orbit** [2341, 2906, 3541]. **spin-polarized** [2130]. **spin-spin** [3541]. **Spin-Unrestricted** [796]. **Spin-Waves** [816]. **spinless** [547]. **spinor** [3709, 1385, 1604]. **Spinors** [1166]. **spiral** [2053, 1441]. **spiraling** [2504]. **Spiro** [942]. **Spiroconjugation** [942]. **spirographs** [57, 205]. **spirosuccinimide** [1323]. **Spline** [3650, 3391, 374, 2481, 3726, 3159, 3450, 3508, 2201, 3125, 3304, 3572, 3197]. **Spline-based** [3391]. **spline-fitting** [2201]. **spline-in-tension** [3450]. **splines** [3105, 3017, 3607, 3322]. **Split** [1826, 3446, 3309]. **Splitting** [3697, 3066, 3113, 2698]. **Sponge** [1130]. **spots** [3451, 2279]. **spread** [1192]. **spreading** [2179, 3469]. **Spring** [873]. **Springer** [759]. **spurious** [1389, 2701]. **Square** [1128, 706, 1906, 2187, 201, 284, 1237, 3425, 300].

square-root [201]. **Squared** [835, 891, 881]. **squares** [2534, 1770, 1533, 539, 2591, 2399]. **squarified** [2695, 2888]. **squeezes** [1201]. **Sr** [1513]. **Stabilities** [1169]. **Stability** [3023, 1807, 3658, 834, 3019, 1505, 1023, 3436, 1242, 1292, 3665, 1583, 3619, 2553, 2741, 2761, 2516, 2815, 3325, 3135, 3519, 2767, 2973, 2798, 2909, 3264, 3231, 2159, 3110, 2281, 3268, 3280, 3349, 989, 695, 1302, 3638, 1238, 3351, 3279, 2061, 2803, 2816, 1688, 1732, 3317]. **stability-aromaticity** [1688]. **stabilizing** [3711]. **Stable** [817, 3400, 906, 755, 2892, 2337, 3325, 1498, 3335, 3378, 3480, 3471, 3450, 3364, 3300, 3302, 3316, 3508, 3199, 637, 3370, 3426, 2461, 2462, 1084]. **stacking** [3688]. **stage** [1479, 2566, 2207, 3064, 2594, 3271]. **stages** [2673, 2691, 2709, 2938, 2908, 3039, 2991, 2746, 2922, 3012, 2798, 2960, 2633, 2856, 2733, 2855, 3037, 1269, 2844, 2971, 2648, 2994, 2876]. **staggered** [445, 517]. **Staircase** [703]. **standard** [1047, 1677, 1684]. **stannates** [2506]. **Star** [2012, 2243, 1100]. **star-branched** [1100]. **starburst** [565]. **Stark** [661]. **stars** [3180]. **starting** [1971, 2295]. **State** [898, 861, 926, 2259, 821, 864, 902, 401, 833, 825, 2180, 2068, 2669, 3501, 2403, 718, 2772, 1926, 3344, 2016, 2043, 3413, 481, 740, 1291, 1362, 1277, 291, 3182, 2162, 2181, 3048, 2492, 319, 2075, 2884, 2564, 2688, 2011, 2427, 1552, 3282, 1995, 1003, 972, 1765, 167, 534, 3418, 658, 2044, 3041, 3308, 2583, 852, 1966, 2062, 2680, 2238, 33, 2056, 437, 1704, 1235, 2639, 2145, 1307, 249, 1999, 1386, 3136, 51, 1266, 3237, 2347, 616, 2267, 2175, 1534, 1862, 2459, 1784, 2671, 3348, 2697, 2853, 1658, 1044, 1054, 2460]. **State-Universal** [902]. **States** [866, 841, 911, 240, 1870, 3587, 2068, 3123, 3339, 1971, 3094, 3204, 3709, 2316, 2951, 1280, 1556, 1514, 2367, 2986, 2249, 1875, 283, 2362, 304, 3507, 2042, 1133, 1047, 3579, 276, 278, 1394, 125, 96, 1518, 2365, 2275, 2552, 2713, 3289, 3512, 3566, 2108, 2497, 2619, 2836, 1344, 2429, 51, 3506, 2703, 1941, 973, 489, 671]. **static** [3068, 3348]. **Stationarity** [2175]. **Stationary** [2124, 743, 1875, 1873, 2349, 2836, 48, 1829]. **Statistical** [940, 1324, 2137, 888, 2163, 1613, 347, 3245, 2705, 2006, 1352, 3558, 1206, 1900, 2879, 598, 3634, 2464, 2307, 2394, 101, 3650, 3607, 3366, 343, 1465, 1466, 1634, 686, 3644, 2092, 2430]. **statistical-like** [3634]. **Statistical-mechanical** [1613]. **statistically** [3445]. **Statistics** [619, 27, 2906, 1305, 2443, 535, 2164, 2864, 642, 2440, 1400, 2441]. **Staying** [3432]. **steadily** [2327]. **Steady** [3604, 2492, 2259, 3136, 3237, 833, 3587, 2316, 2403, 1926, 3344, 2249, 291, 2181, 3048, 319, 2884, 2011, 2427, 3282, 3507, 1995, 1003, 3579, 2583, 2238, 1704, 1307, 1999, 1386, 51, 2347, 1862]. **Steady-state** [2492, 3136, 3237, 319, 1995, 1704, 1307, 1999, 1386, 1862]. **Steffensen** [3516]. **Steffensen-like** [3516]. **Steinborn** [1459, 1460]. **STEM** [3018]. **stents** [2621]. **Step** [1136, 814, 3400, 1628, 1798, 1871, 2060, 2029, 2118, 2178, 2253, 2392, 2410, 2322, 2544, 2549, 2472, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 2938, 2908, 1479, 2759, 3493, 2255, 2764, 2734, 2746, 3247, 2922, 2999, 3504, 3696, 3325, 2943, 3012, 2566, 3005, 1633, 1695, 2778, 2935, 2909, 2576, 2541, 2725, 2633, 3378, 3480, 3471, 2847, 3109, 2733, 2851, 2855,

3278, 3364, 3300, 3268, 3280, 3302, 3316, 3497, 3548, 3586, 3459, 3508, 2507, 175, 1525, 2213, 1540, 3435, 3569, 3199, 1101, 1355, 1904, 2098, 2317, 2381, 2370, 2455, 3406, 2930, 3370, 3426, 3707, 3081, 963, 2971, 3033, 2648]. **step** [3044, 2914, 2876, 2834, 2594]. **step-point** [1540]. **step-size** [3435]. **Steps** [832, 2330, 2485, 1602, 3294, 2541, 2499, 2725, 1573, 694, 357]. **steps-** [694]. **stepsize** [1684]. **stepwise** [12, 166, 3047]. **stereo** [2363]. **stereo-isomers** [2363]. **stereochemical** [1229, 2358, 155]. **Stereochemistry** [820, 850, 904, 351, 2048, 2049]. **stereodescriptors** [2452]. **stereodynamics** [2743]. **stereogenic** [2452]. **Stereogenicity** [850, 904, 2027, 2028, 2451, 2451]. **Stereogenicity/Astereogenicity** [850]. **stereogenicity/RS** [2028]. **stereogenicity/stereoisomerism** [2028]. **stereographs** [155]. **stereoisogram** [2048, 2298, 2299, 2371, 2372, 2358]. **Stereoisograms** [2027, 2028, 2450, 2451, 2452, 3456, 3457, 3468, 1585]. **stereoisomeric** [2048, 3456, 3457, 3468, 2450]. **stereoisomerism** [1761, 2028]. **Stereoisomers** [1173, 1154, 991, 1585, 2298, 2585, 1811, 2299, 2371, 2372, 2584]. **stereoselection** [71]. **stereoselectivity** [3514]. **stereoskeletons** [2491]. **Stern** [3070]. **Sternberg** [552]. **Stieltjes** [2854]. **stiff** [3564, 1891, 3170, 3513, 3435, 1234, 3406, 1322, 1358]. **Stiffness** [873]. **Still** [875]. **Stirred** [802, 2964, 699, 738]. **stirred-tank** [699]. **STO** [1167]. **Stochastic** [1713, 774, 1408, 2470, 3286, 2518, 714, 2210, 2152, 2114, 2418, 3048, 3043, 455, 2312, 2173, 2223, 1568, 1626, 2014, 2105, 3377, 1372, 2788, 3405, 2737, 2422, 2356, 3656, 2354, 2610, 3597, 3212]. **stochasticity** [3176]. **Stockholder** [1476, 1622]. **stoichiometric** [3121]. **stoichiometry** [715]. **Stone** [3345]. **STOs** [2600, 1160]. **stranded** [2070]. **strategies** [1924, 394]. **strategy** [1094, 2944, 279, 280, 666, 2331]. **Stratospheric** [1360]. **strength** [683, 725]. **Strengths** [3206, 3205, 3576]. **streptokinase** [1191]. **Stretching** [844]. **strictly** [131]. **String** [160, 1411]. **strings** [93]. **Strip** [1128, 3013]. **strips** [2672, 3127]. **strong** [691, 1049, 1743]. **Strongly** [96, 1941, 3007, 3579, 3151, 3398]. **strongly-damped** [3151]. **strontium** [2506]. **Structural** [2560, 803, 947, 2436, 2357, 2923, 2535, 3655, 182, 1204, 551, 218, 626, 3209, 2315, 30, 31, 2919]. **Structurally** [786, 2000]. **Structure** [472, 856, 915, 896, 1128, 916, 1701, 1105, 1149, 658, 1075, 907, 933, 2804, 25, 91, 1763, 3201, 567, 2827, 193, 984, 1288, 1351, 2984, 3255, 3634, 471, 581, 2420, 80, 225, 1423, 319, 1530, 231, 2598, 1447, 2831, 1951, 3062, 3464, 196, 341, 1497, 1390, 2134, 1327, 153, 128, 165, 2531, 2786, 3460, 2897, 233, 246, 2144, 1432, 1382, 1622, 2104, 3623, 1204, 258, 2469, 551, 583, 2791, 90, 3555, 73, 1583, 3505, 1934, 392, 1076, 322, 459, 3236, 2640, 1539, 2133, 1102, 3732, 2745, 1520, 1783, 3630]. **structure-activity** [1763, 319, 2831, 128, 165, 3460, 3623, 2133]. **structure-based** [1497]. **structure-preserving** [3062, 2531, 2897, 3732]. **structure-properties** [471]. **structure-property** [233, 1539]. **Structure/formula** [1701]. **structured** [1811, 2631, 1378]. **Structures** [1010, 846, 811, 1158, 2654, 638, 3053, 1916, 1279, 3734, 1897, 41, 721, 1037, 1103, 740, 2131, 1646, 1417, 3182, 361, 2063,

109, 110, 161, 991, 227, 1363, 265, 155, 589, 3087, 2863, 1207, 1180, 2721, 1441, 3521, 1349, 166, 994, 75, 2838, 3380, 956, 1438, 2061, 274, 2107]. **studied** [1411]. **Studies** [1106, 1577, 3245, 665, 1970, 1763, 2071, 744, 1206, 248, 165, 1587, 43, 3654, 1430, 3146, 686, 3527, 3625, 1844, 3629, 2323, 3047, 961]. **Study** [3641, 186, 3388, 1276, 1231, 798, 1340, 3647, 2068, 2705, 2875, 329, 2433, 3083, 3288, 951, 1324, 2290, 193, 1202, 2572, 2670, 3331, 3498, 2516, 2225, 88, 2513, 2448, 266, 3607, 10, 1685, 3460, 1801, 1667, 2788, 2656, 2718, 513, 514, 593, 2208, 2439, 533, 3209, 1691, 1100, 1323, 3371, 1911, 2116, 2348, 2641, 739, 3537, 3638, 3704, 1534, 3705, 636, 701, 2687, 1939, 1409, 1688, 1544, 1547, 1694, 2487]. **studying** [3114, 3519, 3630]. **Sturm** [2231, 2082, 1068]. **Sturmian** [618, 708, 851, 2605]. **Sturmians** [549, 691, 2287]. **styrene** [1981]. **sub** [2100]. **subclass** [2526]. **subdiffusion** [3682, 3603]. **subdivision** [3053]. **Subduced** [780, 929, 109, 2049]. **Subduction** [110, 109]. **Subductions** [929]. **Subgraph** [446, 1016]. **Subgraph-driven** [446]. **Subgraphs** [1424, 81, 229, 1539]. **Subgroup** [770, 2586, 3456]. **subgroups** [3339, 421]. **subject** [1556, 3323, 3590, 1404]. **subnetworks** [1985, 131]. **suboptimal** [2292]. **subsequent** [1753]. **subset** [1694]. **subspace** [1850, 1647]. **Subspaces** [905, 2814, 1501, 459]. **subspectral** [86]. **Substance** [1061]. **substances** [2772, 1564, 1601]. **Substituent** [768, 106]. **substituents** [118, 3625]. **substituted** [1615]. **Substitution** [872, 1134, 2237, 2587, 1579]. **Substitution-Reaction** [1134]. **substitutional** [2088, 2100]. **Substrate** [901, 2095, 903, 3344, 2999, 2181, 3609, 3668, 3011, 2250, 1704, 2819, 1356, 1373, 1386, 1606, 1240, 1231]. **Substrates** [833, 1853, 2002, 2882, 698]. **substructure** [546]. **substructures** [161]. **subsystem** [467]. **subsystems** [1629]. **successful** [3504]. **Sudden** [3415, 3590]. **sufficiency** [564]. **Sufficient** [372, 660]. **Suggested** [911, 973, 1703]. **suicide** [2002]. **suitably** [1952]. **sulfonamides** [1200]. **sulfur** [1841]. **sulphur** [1717, 2073, 2115, 2295, 2489, 2515, 2711]. **Sum** [401, 1720, 3399, 2504, 3183, 1728, 1631, 3553, 3175, 3522, 1590]. **Sum-connectivity** [1720, 3399, 1728, 1631, 1590]. **Summary** [277]. **summation** [334, 456, 3126, 3657]. **summations** [613]. **sums** [3188]. **Super** [2726, 3450, 1523, 1809, 1758, 3508]. **Super-stable** [3450, 3508]. **super-symmetric** [1758]. **superaromatic** [492]. **Superboson** [811]. **superconductivity** [498]. **superconductors** [3169]. **Superconvergent** [797]. **supercooled** [712]. **superdiffusion** [2980]. **superhard** [981]. **superheavy** [3094]. **superhelix** [311]. **superposition** [747, 513, 514, 593, 1790, 2703]. **supersaturated** [2571]. **supersaturation** [2963, 3615]. **superselection** [130]. **Superspherical** [1918]. **Superspherical-shape** [1918]. **Supersymmetric** [1019, 1156, 2365, 2275, 2360, 2554]. **Supersymmetry** [1570]. **supplies** [3609]. **support** [2700, 1801, 1739, 2883]. **Supported** [861, 2348, 2467, 2561, 2641, 3153, 3256, 1981]. **supposing** [3236]. **suppressed** [3205]. **suppressing** [2701]. **suppression** [3500, 3570].

supratransmission [2989]. **supreme** [3604]. **Surface** [880, 834, 793, 937, 1032, 2588, 906, 2800, 1744, 2304, 1946, 1545, 515, 723, 724, 1531, 426, 427, 3403, 345, 3675, 2041, 2857, 219, 20, 150, 2116, 3153, 2957, 1409, 3144, 1285, 3211, 385, 599, 2883, 2743, 727]. **Surfaces** [793, 1086, 3395, 3105, 52, 520, 1393, 2765, 46, 3322, 1836, 1873, 43, 3045, 1944, 418, 1911, 2116, 2194, 2924, 382]. **surfaces-applications** [1393]. **Surfactant** [2247, 1856, 1935]. **Surfactants** [943, 2800, 1768]. **Surpassing** [900]. **Surrogate** [3374]. **surrounded** [558]. **survey** [1508, 981]. **Survival** [2343, 2254, 2952]. **surviving** [2344]. **susceptibility** [70, 1378]. **suspicious** [2071]. **sustainable** [3628]. **sustaining** [2536]. **SUSY** [2144]. **SUSYQM** [3267]. **swapping** [703]. **swarms** [2665]. **sweep** [707]. **swelling** [3007, 2693]. **Swerdlow** [2430]. **Swift** [3257]. **switch** [2170, 1946]. **SWKB** [762, 1614]. **Symbolic** [1541, 2017, 2018, 2401]. **symbols** [334, 456, 135]. **Symmetric** [3339, 585, 800, 863, 911, 1137, 324, 832, 2595, 2673, 2623, 2691, 2709, 2938, 2908, 2514, 3051, 3224, 2746, 2016, 2136, 2922, 2304, 2848, 1019, 1156, 2414, 2943, 2566, 3127, 2935, 1425, 1758, 2633, 2856, 3528, 2214, 1525, 2213, 8, 2429, 2930, 663, 2530, 2023, 482, 2648, 2914, 2698, 2594, 1247]. **Symmetric-group-based** [585]. **Symmetrical** [1953, 1595, 1769, 3462, 2347]. **Symmetries** [910, 1173, 3020, 770, 1998, 1119, 2288, 2685, 3115, 3360, 1828, 3357, 3016, 3052, 3667, 3112, 525, 1155, 1251, 1330, 1293, 2487]. **symmetrized** [592]. **Symmetry** [2373, 3428, 1393, 850, 2298, 2299, 2371, 2372, 60, 632, 2047, 2113, 770, 3189, 3210, 893, 3321, 1089, 2804, 330, 681, 2435, 3337, 3532, 213, 212, 2448, 2490, 2820, 3496, 1761, 512, 2710, 318, 589, 1426, 3151, 99, 582, 2285, 1332, 572, 592, 2100, 2666, 653, 526, 670, 1949, 2550, 2230, 614, 3622, 1662, 2239, 2805, 1694, 2450]. **Symmetry-adapted** [2373, 1393, 2047, 3210, 2435, 2710]. **Symmetry-breaking** [2113, 1332]. **symmetry-distinct** [1426]. **Symmetry-itemized** [2298, 2299, 2371, 2372, 2450]. **Symmorphy** [409]. **Symmtry** [3145]. **Symmtry-itemized** [3145]. **Symplectic** [1116, 1174, 867, 889, 1062, 1956, 2848, 953, 541, 964, 1098, 2024, 1043, 1993]. **synaptic** [11]. **Synergism** [2740]. **synergistic** [1853, 3340]. **synisometry** [2547]. **syntheses** [717, 715]. **Synthesis** [1152, 1916, 1713, 3307, 2321, 1509, 3494, 54, 2166, 2506, 2946]. **Synthesising** [2444]. **synthetic** [3502, 3718]. **synthon** [53, 54]. **System** [1034, 939, 1187, 1136, 1032, 1027, 1016, 749, 798, 825, 3123, 2712, 3196, 3118, 2124, 3565, 3323, 1472, 675, 1740, 3589, 316, 550, 2884, 1690, 1679, 296, 1552, 60, 953, 1057, 377, 1198, 2359, 948, 151, 128, 165, 2611, 1242, 2228, 2177, 2199, 2313, 2559, 2628, 2615, 3140, 1292, 1564, 2505, 3528, 2974, 1350, 1456, 1599, 1600, 1618, 641, 33, 3368, 3367, 2285, 2980, 1734, 3388, 507, 2707, 2675, 2818, 1725, 1721, 3595, 2262, 518, 2987, 3359, 3239, 497, 993, 1407, 1414, 3467, 3584, 1974, 1371, 682, 3095, 3454, 2061, 430, 484, 482, 1997, 2065, 2425, 2577, 2745, 2912, 3348, 1044, 1054, 1253]. **system** [463]. **Systematic** [2091, 991, 10, 1204, 306]. **Systematically** [2473]. **Systems**

[890, 842, 838, 888, 920, 1151, 772, 885, 926, 1029, 854, 1073, 1018, 1084, 798, 823, 3106, 2437, 3587, 3023, 1896, 3168, 1352, 1858, 2453, 3184, 975, 1849, 3224, 2741, 3432, 1607, 3250, 467, 2777, 2357, 360, 2249, 501, 502, 523, 543, 3115, 2329, 743, 3226, 3050, 1567, 295, 2812, 2294, 2516, 3535, 3103, 1961, 1962, 2090, 224, 1214, 2848, 709, 606, 283, 2276, 2448, 2996, 528, 2939, 2564, 2688, 3424, 2535, 2017, 2018, 2368, 2369, 2664, 2625, 2186, 431, 3270, 3336, 1244, 115, 3079, 3228, 3342, 3507, 1889, 3610, 2312, 2173, 2223, 3727].
systems
[2139, 2401, 3593, 3309, 3516, 138, 2767, 3170, 2985, 3618, 2531, 3034, 3726, 3725, 1531, 1775, 3360, 97, 332, 363, 3221, 3377, 3702, 1428, 343, 2128, 2129, 2342, 2545, 3588, 3055, 3513, 689, 2127, 2126, 2306, 2925, 1215, 2141, 513, 1349, 1354, 1235, 1787, 1802, 2690, 1036, 2989, 1455, 2676, 235, 3373, 2474, 1378, 3435, 2405, 3213, 1859, 2729, 73, 1290, 2416, 2822, 2536, 3249, 634, 2175, 1616, 3705, 537, 2212, 2458, 3649, 2233, 116, 1756, 1193, 591, 2239, 2723, 694, 522, 560, 622, 111, 211, 1322, 1358, 1330, 1649, 2083, 1446, 1759, 2792].

T [2602, 692]. **T-hull** [692]. **Table** [826, 3094, 181, 80, 730, 3128]. **Tableaus** [3339]. **tables** [2150]. **tackling** [3586]. **Tagged** [597, 568]. **Takens** [2577]. **taking** [2802]. **Tamm** [2445]. **Tangent** [881]. **Tanimoto** [1698, 679, 3703]. **Tank** [802, 2964, 699, 738]. **target** [3417, 1127]. **targeted** [1875]. **targeting** [3401]. **targets** [3503, 3576, 3542]. **tartaric** [991]. **tautomerism** [2781]. **taxol** [440]. **Taylor** [1777, 1805, 3057, 3084, 3513, 3249, 2799]. **TB** [1092]. **TB-curve** [1092]. **TBP** [2906]. **TDDFT** [1612]. **TDRK** [2522]. **tea** [3675]. **technicalities** [2748]. **Technique** [1142, 3114, 3193, 2005, 2154, 2597, 1472, 169, 83, 2496, 3036, 3567, 3363, 3369, 3681, 566, 661, 2144, 2214, 542, 3669, 3595, 3672, 2389, 2581, 3167, 3467, 3693, 3266, 3677, 622]. **Techniques** [1020, 777, 1152, 2158, 3686, 2995, 1800, 2120, 481, 1947, 2754]. **technology** [3222]. **teeming** [3037]. **Telegraph** [3650]. **telescope** [2695, 2888]. **telescopic** [2320]. **Teller** [2653, 2906, 3694, 3323, 417, 2093, 2671]. **Teller-like** [2093]. **Teller-type** [2671]. **Temperature** [2102, 2521, 159, 1835, 1208, 3285, 2553, 2732, 1256, 1297, 1729, 1530, 955, 2442, 2854]. **Temperature-time** [1835]. **temperatures** [3184, 2506, 3169]. **templator** [3237]. **Temple** [900, 1959, 2222]. **tempo** [261]. **temporal** [2162, 3653]. **Ten** [311, 1871]. **ten-step** [1871]. **Tension** [1032, 3607, 2588, 3450, 1409]. **tensor** [2015, 1915, 97, 332, 363, 1722, 322]. **Tensorial** [3190, 811, 204, 476, 696, 697]. **tensors** [395, 366, 532]. **tenth** [2673, 2691]. **Term** [768, 2032, 1777, 3660, 1729, 3303, 3178, 3447, 1882, 2360, 3444, 2300]. **Terminal** [1517]. **terminated** [1546]. **terminology** [2358]. **Terms** [1179, 931, 3106, 2264, 1955, 3583, 204, 658, 852, 406, 40, 946, 2992, 3128, 133]. **ternary** [1069]. **Tessellations** [1010, 3475, 658]. **Tessier** [1504]. **Tessiet** [1373, 1317]. **test** [1634, 3434]. **tested** [406]. **testing** [2776]. **Tests** [1535, 158]. **Tetra** [1155, 199]. **tetra-atomic** [199]. **Tetra-halide** [1155]. **tetrahedra** [2366, 2650]. **Tetrahedral** [1115, 2435, 1895]. **tetramethyl** [1102]. **tetrapod** [1432]. **tetrathia** [2587]. **Tetratomic** [906]. **TGA** [1175].

th [685, 3023, 1202, 3122, 1498, 806, 1843]. **th-order** [1202]. **THDRK** [3030]. **Their** [857, 792, 790, 306, 2595, 3168, 259, 61, 2696, 2928, 3710, 2952, 1113, 3201, 3207, 1163, 3634, 3372, 3142, 3111, 2160, 2190, 2728, 2243, 2535, 2017, 3553, 60, 1014, 1050, 1167, 1205, 1246, 1284, 1737, 3519, 256, 10, 2972, 1180, 1712, 1372, 1382, 1623, 2008, 2269, 419, 508, 1964, 1365, 3093, 1290, 1993, 31, 506, 3629, 245, 998, 1172, 1364, 560, 622, 1119, 1201, 1155, 1251, 1293, 780]. **themselves** [3557]. **Theorem** [330, 329, 331, 884, 883, 2573, 2237, 866, 784, 1028, 3617, 728, 1666, 3120, 348, 2309, 975, 678, 1865, 362, 1744, 1805, 2176, 2782, 2689, 3275, 3549, 2121, 628, 2394, 2319, 206, 407, 278, 103, 209, 2261, 1039, 18, 650, 285, 2083, 2731, 2657]. **Theorems** [466, 1014, 268, 1033, 1942, 140, 1050, 1205, 1284, 1447, 1595, 1659, 1769, 336, 1185, 1907]. **theoretic** [1508, 1681, 1812, 979, 94, 2509, 2087, 2179, 3469, 507, 1635, 2532, 3458]. **Theoretical** [1208, 2976, 2587, 3233, 2420, 3096, 780, 820, 3494, 2208, 3523, 2992, 3506, 3612, 451, 634, 3613, 2632, 244, 3646, 2111, 471, 411, 1961, 88, 434, 1173, 1741, 1327, 162, 58, 124, 3366, 2030, 317, 642, 104, 683, 249, 2246, 3663, 2098, 666, 2674, 210, 1409, 1673, 2854, 494]. **theories** [2940, 244, 1669, 1668, 2951, 3542, 245, 1285]. **Theory** [882, 1126, 925, 1070, 24, 838, 1761, 455, 1151, 1468, 1664, 2899, 1921, 22, 723, 1067, 426, 125, 2198, 1068, 2819, 3176, 795, 897, 552, 797, 3683, 240, 3161, 1628, 2463, 728, 1258, 1992, 2074, 52, 974, 386, 2406, 174, 2309, 2906, 3409, 2012, 397, 564, 367, 114, 2357, 1945, 981, 2202, 690, 2614, 334, 1804, 1796, 2555, 2089, 2090, 2898, 1040, 50, 3137, 2276, 2490, 3438, 3352, 1887, 2695, 2888, 3544, 1929, 1366, 1595, 1604, 407, 1714, 1096, 1765, 4, 5, 284, 2913, 165, 504, 1001, 3347, 276, 527, 1200, 2426]. **theory** [2863, 2117, 2128, 2129, 2342, 2545, 119, 1380, 3547, 3522, 3314, 2407, 2360, 1667, 3654, 2867, 1851, 2094, 175, 3416, 1382, 1448, 1452, 1445, 1624, 1623, 2104, 70, 635, 1455, 1300, 704, 8, 2666, 2753, 2948, 616, 497, 739, 3741, 3, 1532, 2521, 3121, 560, 1835, 1694, 106, 3630, 671, 2900]. **theory-based** [165]. **therapeutics** [3646]. **therapy** [1668, 2071]. **there** [1926, 577]. **Thermal** [1908, 1080, 2843, 3126, 3367, 1628, 3721, 2479, 2860, 2617, 2449, 3669, 2263, 3119, 2157, 2233, 2340, 3414, 2471, 3568, 3368]. **thermal-average** [2449]. **thermalization** [624]. **Thermochemical** [423, 94]. **Thermodynamic** [2781, 331, 2311, 1607, 114, 2571, 1963, 3135, 2361, 1613, 3416, 2382, 3388, 3246, 478, 3394, 2459, 2460, 3671]. **Thermodynamical** [3659, 2294]. **Thermodynamically** [2462, 2461]. **thermodynamics** [2403, 2516, 3137, 2793, 420, 2235, 2182, 1648, 33, 735, 1487]. **thermoelastic** [3506, 3612]. **thermokinetics** [1283]. **thermostability** [2441, 2440]. **Thermostat** [1083]. **therodynamic** [457]. **thiazolyl** [1621]. **thick** [1592]. **thickness** [3070]. **thin** [3713, 3065, 2694, 3016, 1767, 1402]. **thioethers** [3494]. **Third** [3508, 1217, 3624, 2178, 2410, 2544, 2524, 2549, 2472, 2623, 2662, 2709, 1994, 3378, 2733, 2507, 2511, 324, 2723, 1772, 2594]. **third-order** [324, 2723]. **Thirty** [312]. **Thomas** [338, 655, 189]. **Thompson** [1843]. **Thomson** [528, 2717]. **thought** [2111, 359]. **Thoughts** [1400]. **Three**

[1114, 898, 3375, 2746, 834, 3361, 2519, 2358, 2243, 1014, 1022, 872, 84, 699, 758, 877, 2561, 2957, 921, 3338, 2130, 2908, 3385, 1858, 1359, 3542, 66, 122, 408, 1346, 1868, 2922, 435, 169, 2996, 2688, 991, 1229, 2450, 2451, 2452, 3456, 3457, 3468, 3240, 299, 3091, 1007, 342, 3618, 2652, 1599, 1600, 3450, 2855, 3037, 2174, 156, 257, 2980, 1261, 3669, 1540, 3423, 3435, 573, 1491, 2627, 3584, 3362, 1302, 537, 1222, 1823, 1409, 3556, 2471, 3211, 347, 522, 622, 1387, 3222, 1488]. **three-** [2688]. **three-agent** [2980]. **three-body** [3542, 408, 3091, 2174]. **Three-Center** [758, 1014, 1599, 1600, 1261, 3362]. **three-component** [3584]. **three-coordinated** [3618]. **Three-Dimensional** [877, 3361, 2243, 84, 66, 122, 435, 169, 991, 1229, 1007, 156, 3669, 1302, 537, 3211, 347, 522, 622, 1387, 3222]. **three-electron** [2130, 1868, 2652, 2627, 1488]. **three-exponential** [1858]. **three-fold** [342]. **Three-layered** [2957]. **three-membered** [2450, 2451, 2452, 3456, 3457, 3468]. **Three-particle** [2519]. **three-species** [3385]. **three-spin** [2996]. **three-stages** [2908, 2922, 2855, 3037]. **Three-State** [898]. **Three-Way** [921]. **Threshold** [2737, 2677]. **through-bond** [1428]. **through-bridge** [1787, 1776]. **Through-space** [1776]. **throughput** [1127]. **Ti** [3641]. **Tietz** [2227, 2941, 2352]. **tight** [1546]. **tight-binding** [1546]. **Tikhonov** [752, 1799]. **tiles** [2862]. **tilings** [1646]. **tilt** [672]. **Tilting** [673]. **Time** [862, 3206, 778, 916, 2665, 3383, 1533, 888, 772, 1174, 2512, 2604, 983, 3051, 1389, 1453, 2431, 2741, 2740, 2842, 3083, 3205, 3500, 3538, 3570, 3697, 3565, 2866, 3673, 2858, 3255, 3323, 2636, 3142, 3598, 2114, 3404, 2841, 2944, 2165, 2168, 3676, 3455, 1780, 2447, 1316, 1190, 1741, 1216, 3567, 3645, 965, 658, 3397, 3653, 1568, 1626, 2169, 2184, 2419, 3682, 2896, 2281, 1584, 2488, 3332, 3354, 3388, 3476, 2046, 2675, 2232, 2405, 2979, 1678, 3509, 3603, 2429, 2351, 3552, 3573, 2618, 3405, 3695, 1766, 2703, 3677, 3622, 3279, 1193, 3546, 2616, 389, 390, 1835, 1044, 1054, 1446]. **Time-dependent** [3383, 2512, 2604, 3565, 3397, 2169, 2184, 2419, 2896, 2281, 3354, 3476, 1678, 389, 390, 1044]. **time-fractional** [3673, 3404, 3676, 3567, 3653, 2488, 3509, 3603, 3677, 3546]. **Time-independent** [1174, 1054, 1446]. **time-integration** [3279]. **time-like** [3142]. **time-of-flight** [2488]. **Time-property** [1533]. **times** [1553, 1310, 1317, 1340]. **timescales** [3373]. **timing** [3443]. **tissue** [3422]. **titanium** [1922]. **Tm** [2229, 2385]. **Toeplitz** [3224, 3062, 3464, 3477, 2251]. **tolerance** [1549]. **TOMOCOMD** [1372, 1380]. **tool** [1927, 1324, 3553, 2340, 2273]. **Tools** [778, 780, 183, 789, 1673, 2476, 116]. **top** [1477]. **Topographical** [1652, 1672]. **Topography** [2041]. **Topological** [2993, 3053, 722, 216, 1163, 579, 304, 3475, 3445, 2543, 1169, 157, 3515, 357, 454, 2505, 45, 307, 2094, 184, 3550, 1056, 1059, 905, 830, 3419, 1571, 1147, 3317, 3338, 3624, 2663, 2965, 3484, 1916, 2444, 208, 260, 261, 1037, 1103, 3104, 3449, 1351, 286, 3631, 207, 50, 1252, 186, 6, 2500, 3578, 3626, 1005, 947, 1591, 340, 305, 266, 2882, 84, 321, 2681, 2628, 3029, 693, 302, 47, 3644, 3003, 3052, 306, 1473, 2459, 2461, 2460, 2462, 2706, 1539, 3013, 1397, 1342]. **topologically** [37, 251, 387, 371, 1409]. **topologies** [346]. **Topology**

[792, 1432, 573, 330, 1493, 271, 2292, 2473, 2235, 2182, 4, 5, 22, 13, 284, 589, 586, 1425, 1426, 345, 272]. **topology-driven** [1426]. **tori** [2722, 1420, 1431, 3357, 1438]. **toric** [3173, 3531]. **Toroidal** [1359, 2542, 1012, 2726, 2569, 2790, 3263, 1249, 1345, 2784]. **toroids** [1428]. **torque** [1949]. **torquoselectivity** [3514, 524]. **Torricelli** [2650]. **Torsion** [819, 1663, 2013, 469]. **torsional** [1670]. **Torus** [1108, 2374, 2377, 1304, 2107, 2052]. **Torvik** [3054]. **Total** [3132, 2870, 329, 2842, 2203, 3344, 1987, 2020, 1262, 2789, 1006, 189, 1210, 1365, 2331, 2236]. **Toxic** [1301, 1564]. **toxicity** [1361, 266]. **Toxicological** [789]. **toxin** [1053, 1183]. **TPD** [1069]. **TPD-CO** [1069]. **trabeculate** [3171]. **traceability** [81]. **Trajectories** [1107, 937, 941, 1896, 953, 1873, 2041, 2590]. **trajectory** [135, 2743]. **trans** [2539, 2948]. **trans/cis** [2948]. **trans/cis-** [2948]. **transactinide** [3094]. **transcendental** [3474, 1493, 2560]. **transcriptase** [3627]. **transcription** [3176, 3332]. **transduction** [1307, 704]. **Transfer** [1020, 1309, 2732, 3442, 3441, 3685, 467, 675, 2684, 1950, 2126, 2140, 514, 2252, 2484, 249, 2758, 594, 700, 2092, 615, 1866]. **transferable** [1546]. **transfinite** [3076]. **Transform** [1085, 1034, 836, 1081, 1160, 1972, 2010, 1453, 1454, 2608, 2579, 2602, 2794, 2702, 2809, 2967, 3083, 3320, 3358, 3538, 3604, 3570, 3720, 3697, 990, 3353, 335, 2468, 121, 3299, 1483, 2639, 1482, 2399, 1641, 3235, 3412, 2232, 1520]. **Transformation** [2983, 1165, 259, 2387, 3004, 424, 640, 563, 2360, 175, 1670, 1784, 65, 318]. **Transformations** [1072, 409, 1953, 289, 2642, 439, 464, 490, 692, 651, 1837, 380, 961]. **transformed** [2419, 2281]. **Transforming** [1698]. **transforms** [386, 996, 2464, 1038, 2336, 2416]. **Transient** [2437, 1204, 1011, 2679, 2488, 712, 652]. **transients** [1955]. **Transition** [861, 2687, 638, 2357, 740, 1530, 161, 3035, 1765, 2044, 96, 2102, 2206, 1766, 1988, 1534]. **Transition-metal** [2687]. **Transitions** [898, 1945, 2739, 674, 2198, 1411, 1522, 1694]. **transitive** [4]. **Translation** [1061, 3309]. **translational** [2747]. **Translationally** [3127]. **translations** [442]. **translator** [2233]. **transmembrane** [590]. **transmission** [1241, 1618, 2256, 558, 2840, 2428, 3554]. **transport** [1807, 2587, 2376, 1780, 1316, 1190, 1377, 1562, 1660, 1710, 2635, 2811, 448, 1794]. **transversely** [2479]. **trap** [3069]. **trap-free** [3069]. **trapped** [3354, 250, 1620, 1727]. **Trapping** [2101]. **traps** [2292]. **Traveling** [2896, 1718, 1519, 3670]. **Traveling-wave** [2896, 1519]. **Travelling** [550, 874, 518, 450]. **treat** [3631]. **Treatment** [1153, 1870, 2705, 1762, 1792, 283, 3174, 1671, 1205, 1284, 1338, 1385, 1475, 1814, 2208, 2668, 1511, 3695, 1670, 670, 3210, 3098, 2078, 1446, 1759]. **treatments** [135]. **Tree** [27, 85, 543, 2363, 1591, 1811, 1157, 76, 98, 642]. **tree-like** [543, 2363, 642]. **tree-pruning** [85]. **Trees** [1109, 1120, 429, 260, 85, 2696, 2866, 2933, 1631, 9, 1229, 1499, 1005, 1596, 1281, 388, 10, 267, 3230, 3293, 1470, 1211, 2377, 1575, 2289, 2303, 59, 3220,

2076, 123, 1264, 1637, 1720, 1489, 1063]. **Trends** [1685, 2111]. **tri** [1330]. **tri-atomic** [1330]. **trial** [2896, 3227]. **triangle** [37, 1213, 587, 679, 2574]. **triangular** [2161, 3475, 725]. **triangularity** [2160]. **triangulated** [2588]. **triatomic** [2985, 359, 727]. **triazine** [2781]. **Tribonacci** [2852]. **tribopolymerization** [570]. **tribute** [18, 2230]. **tricarbonyl** [88]. **Tridiagonal** [2078, 2777, 2833, 2035, 2401, 3149, 3165, 3223, 3381, 3379, 3477, 3593, 3702, 2707, 349]. **trigger** [497]. **Trigohexagonite** [1738]. **trigonal** [2027, 2028, 3328]. **Trigonometric** [911, 3129, 1982, 3726, 3289, 3304, 973]. **Trigonometrically** [966, 806, 1098, 1174, 2380, 863, 3033, 2853, 1956, 3739, 967, 1099, 1357, 1355, 1993, 2331]. **Trigonometrically-Fitted** [863, 2853, 1956, 3739, 1357, 1355, 2331]. **trihydrogen** [2393]. **trilogy** [2160, 2161, 2162]. **trimethylamine** [739]. **trimolecular** [2422]. **trinomial** [2952]. **triple** [2875, 629, 3571]. **triple-layered** [629]. **Tripling** [1072]. **triply** [1646, 382, 1688]. **Triradicals** [813]. **TRLW** [2582]. **Troesch** [2481]. **truncated** [3639, 3402, 3198, 210]. **Truncating** [1495]. **truncation** [1654, 2160, 2735, 2331]. **truss** [1274]. **Trust** [1105]. **Trust-region** [1105]. **Tsallis** [1465, 1466]. **TSED** [1805]. **TSP** [807]. **Tubercular** [1437]. **tubular** [448, 594, 700]. **tubulenes** [2768, 2846]. **TUC** [1435, 1209]. **tumor** [2602, 3292]. **tumors** [2071, 2651]. **tungsten** [3146]. **tunneling** [3051, 2264, 2840]. **tuples** [277]. **turbidostat** [1552, 1857, 1658]. **turbulent** [2119]. **Turing** [2278, 2724, 1740, 1405, 562, 1823, 3454, 2061, 2988]. **turning** [3681, 3695]. **turnover** [378]. **Tutte** [3075, 3632, 2190, 2664, 2625, 1760, 3213]. **Twelve** [832]. **twin** [3375]. **twist** [1876]. **Twisted** [1086, 1420]. **twisted/chiral** [1420]. **Two** [3124, 3540, 3493, 2995, 678, 1536, 2762, 866, 2893, 895, 920, 1014, 1167, 2248, 822, 1695, 58, 3166, 3400, 887, 804, 2733, 3278, 945, 854, 1027, 1525, 3003, 1491, 1060, 758, 1837, 1011, 3492, 823, 545, 3106, 1628, 2180, 1870, 3123, 2060, 2029, 2673, 2691, 2709, 3738, 918, 1479, 2032, 2759, 1815, 1877, 2951, 3132, 3442, 3441, 3685, 2504, 2124, 3247, 400, 2479, 2739, 2131, 1868, 3598, 2922, 2892, 1602, 3182, 3504, 2283, 3674, 2362, 2642, 2715, 101, 3529, 2187, 3325, 1665, 1483, 1604, 1603, 1737, 1814, 2943, 1889, 3012, 2438, 3091, 2566, 3005, 2359, 965]. **two** [3650, 318, 1633, 2778, 447, 2935, 2909, 2379, 3262, 2541, 2725, 332, 1470, 1828, 2169, 2633, 3378, 3480, 3471, 1884, 3026, 3109, 1350, 1456, 1599, 1600, 852, 1966, 2126, 1723, 1724, 2415, 26, 3364, 3300, 3268, 3280, 3302, 3316, 3497, 3548, 3586, 257, 3368, 3367, 2207, 3508, 575, 372, 2507, 2509, 2690, 1482, 946, 2079, 3251, 1459, 1460, 3290, 2578, 3684, 1721, 2405, 573, 3603, 3573, 3197, 1904, 2389, 654, 3370, 3426, 3707, 2296, 3556, 1411, 1708, 2239, 2971, 1772, 522, 482, 560, 3033, 2648, 3044, 2914, 2835, 2876, 1614, 1314, 2834, 2594, 1903]. **Two-** [1014, 1868, 1604, 3091, 522]. **two-body** [1877, 2379, 332, 2079, 3251]. **Two-boson** [1060]. **two-cell** [2124]. **Two-Center** [920, 854, 1167, 1027, 1491, 545, 1483, 1603, 1737, 1814, 1350, 1456, 1599, 1600, 1482, 946, 1459, 1460]. **two-color** [1314]. **Two-derivative** [2893, 2283, 3674, 3026, 2835]. **Two-Dimensional** [822, 1837, 3738, 918, 1815, 2642, 101, 965, 3650, 447, 3262, 26, 2405, 3603, 2239, 482, 560].

Two-Electron [887, 758, 2951, 3132, 3442, 3441, 3685, 2187, 1889, 318, 2169, 852, 2509, 2690, 654, 1903]. **two-grid** [3573]. **two-layered** [3368, 3367]. **two-mode** [3123]. **two-particle** [2180]. **two-phase** [2479]. **two-photon** [2739]. **Two-point** [3166, 2389]. **two-section** [2296]. **two-stage** [1479, 2207]. **Two-Step** [3400, 3493, 1695, 3278, 1628, 2060, 2029, 1479, 2759, 3247, 3504, 3325, 3012, 2566, 3005, 1633, 2778, 2909, 2541, 2725, 2633, 3378, 3480, 3471, 3109, 3364, 3300, 3268, 3280, 3302, 3316, 3497, 3548, 3586, 3508, 2507, 1904, 3370, 3426, 3707, 2971, 3033, 2648, 3044, 2914, 2876, 2834, 2594]. **two-term** [2032]. **twofold** [2188]. **Type** [890, 2584, 2585, 920, 1017, 1145, 854, 2437, 3124, 3624, 1956, 2178, 2253, 2410, 2322, 1972, 2287, 1457, 1458, 37, 3247, 145, 2593, 1277, 3226, 2418, 3583, 2501, 2456, 3486, 2468, 2597, 2165, 3056, 3698, 2283, 3456, 3457, 3468, 3143, 1321, 1379, 1246, 1338, 1483, 1468, 1471, 1475, 1447, 1595, 1604, 1603, 1737, 2943, 3228, 1481, 201, 2852, 2543, 965, 2132, 3588, 3061, 1350, 1456, 1599, 1600, 1584, 2507, 2819, 1716, 3425, 2145, 1482, 946, 1027, 1310, 1373, 1459, 1460, 3188, 2036, 2975, 1323, 2780, 2810, 3239, 1548, 3362, 1719, 1195, 3274, 2978, 3272, 1238, 1232, 1233, 1594, 1823]. **type** [2868, 2880, 3014, 1254, 1317, 1231, 2723, 1907, 2854, 2671, 2914, 1854, 1278, 3657, 2610, 2692, 2083]. **type-II** [3124]. **Type-itemized** [2584, 2585, 3456, 3457, 3468]. **type-IV** [2584]. **type-V** [2585]. **Types** [1143, 952, 2127, 2126, 232, 3492]. **Typical** [1015]. **Tyrosinase** [1136, 1704].

U [2145, 2123]. **UAH** [3607]. **UAT** [3607]. **UEGO** [2477]. **Ugi** [124]. **Uhlenbeck** [405, 3021, 3656]. **Ulam** [229]. **ultimate** [1440]. **ultra** [2624, 1545]. **ultra-filtration** [2624]. **ultrashort** [2391]. **ultrasonic** [2940, 2912]. **ultrasound** [3184]. **ultraviolet** [2391]. **unambiguously** [3046]. **unbalanced** [3293]. **unbalancedness** [3230]. **unbounded** [2062]. **unbranched** [2330, 2485, 2644, 3022, 224]. **uncertain** [2839]. **uncertainties** [2056]. **Uncertainty** [926, 3720, 2086, 2112, 2383, 1216, 1758, 3377, 3289, 2056, 3388, 1867]. **uncommon** [444]. **uncorrelated** [2148]. **undamped** [3109]. **Undecakisicosahedral** [1182]. **undergoes** [2987]. **underlying** [56, 2910]. **undersampling** [3194]. **understand** [2578]. **Understanding** [223, 3494, 3654]. **understood** [1803]. **Undirected** [354]. **Unequivocal** [1389, 1454]. **Unexpected** [1960]. **Unfixed** [1016]. **unfolding** [1412, 653]. **Unicycle** [1121, 1147, 1230]. **Unicyclic** [753, 1088, 1168, 1048, 1158, 1177, 3238, 1728, 1631, 1270, 1265, 1192, 1189, 1250, 1574]. **unidimensional** [2090]. **unidirectional** [2857]. **unification** [383, 432]. **Unified** [1205, 1338, 1385, 1475, 1814, 1153, 3395, 1284, 2668]. **Uniform** [1785, 3266, 811, 3106, 3361, 1681, 3601, 3391, 1988]. **uniformly** [3681, 3197]. **unifying** [3137]. **unimolecular** [1911, 1711]. **uninuclear** [1229]. **union** [2726, 2222]. **Unique** [890, 1052, 1626, 288]. **Uniqueness** [2321, 784, 1703, 3687, 1905, 1312, 3661]. **Unit** [780, 929, 395, 366, 2983, 2982, 109, 2049, 1441, 7, 2790, 1766]. **Unit-Subduced-Cycle-Index** [780, 2049]. **Unitary**

[2642, 97, 332, 363, 3190, 3191, 3192]. **units** [1646, 252, 2683]. **unity** [2314]. **univariate** [1582, 1778, 1779]. **Universal** [3004, 902, 2316, 2504, 3000, 2204]. **Universality** [1457, 1458]. **universalization** [1696, 1697]. **University** [552]. **unknown** [2534, 3318, 656, 1710, 1714, 1715, 1749, 2025, 1799]. **unnatural** [2859]. **unperturbed** [646]. **unphysical** [240]. **Unraveling** [3529, 2458]. **Unresolved** [418]. **Unrestricted** [796]. **unsaturated** [25, 2247, 745]. **Unsöld** [362]. **unstable** [1352, 1858, 2923]. **Unsteady** [3571, 3669]. **Unsuppressed** [3206]. **unsymmetrical** [1447]. **unusual** [1363]. **updating** [638, 2399]. **upon** [1395, 1123, 3265, 267, 1292]. **Upper** [500, 891, 3080, 737, 1117, 1516, 1262, 1110, 232]. **uptake** [1689]. **USCI** [2049, 2298, 2299, 2371, 2372]. **Use** [231, 999, 1017, 1167, 1246, 1471, 1447, 1764, 2565, 1622, 1790, 2108, 1459, 1460, 1601, 2406, 1202, 2417, 2089, 1421, 1213, 1737, 726, 318, 256, 81, 2365, 2552, 2554, 1382, 3689, 1899, 3622, 3592, 3724, 1542]. **used** [2984, 1872, 3047]. **useful** [639]. **Usefulness** [3119]. **Using** [934, 3193, 752, 836, 917, 938, 1140, 1116, 936, 775, 2900, 758, 3582, 1661, 2940, 1933, 2158, 3023, 2538, 665, 2757, 2287, 1508, 3054, 1922, 168, 1763, 2644, 3086, 2071, 2842, 2809, 2951, 3205, 3206, 3713, 1206, 3658, 2976, 366, 740, 1451, 2636, 2167, 2510, 2624, 3330, 529, 338, 139, 140, 1040, 3483, 435, 169, 3504, 316, 3126, 3324, 83, 1891, 1856, 2862, 3389, 3438, 3479, 2684, 2907, 2936, 3544, 1014, 1091, 1321, 1379, 1483, 1595, 1659, 1769, 3678, 3215, 3334, 1741, 2066, 2059, 2042, 1013, 1811, 1152, 3011, 3516, 3347, 3726, 2480, 427, 2339, 1521]. **using** [1836, 1801, 1033, 1185, 1350, 1456, 1599, 1600, 2261, 2717, 2062, 2306, 257, 692, 2275, 2752, 2788, 3654, 2094, 3485, 3541, 1768, 2080, 2145, 1482, 946, 1329, 3074, 3430, 3267, 3675, 2791, 3412, 1677, 1684, 2232, 1838, 2911, 3346, 3194, 3667, 3552, 3371, 2335, 3058, 3506, 1934, 3426, 1532, 3274, 3249, 3611, 717, 2528, 3162, 2769, 1539, 1767, 2626, 2135, 440, 2300, 482, 64, 65, 3470, 3670, 2891, 1520, 1694, 2441, 2440]. **USR** [2528]. **utility** [2056]. **utilizing** [1853, 3704]. **Uvarov** [2145, 3466, 3267].

V [3468, 1860, 441, 2585, 3457, 111, 211]. **Vacancy** [822, 3345]. **vacuum** [3427, 558]. **Valence** [2877, 278, 446, 1448]. **valence-bond** [1448]. **valences** [1660, 551]. **valent** [342, 586]. **Validated** [756]. **Validation** [2920, 2449, 3607, 3001]. **validity** [3650]. **Valley** [2154, 2041]. **valley-ridge** [2041]. **valleys** [2578]. **valorization** [3558]. **valuation** [715]. **Value** [752, 891, 2908, 2991, 2397, 2406, 1792, 3543, 2922, 2160, 3361, 3483, 3299, 2927, 2943, 2064, 2346, 3369, 3601, 2062, 2680, 2851, 2855, 3243, 1538, 3508, 3147, 3430, 1525, 3235, 2954, 2284, 1386, 1781, 2558, 2638, 2637, 2997, 3281, 3327, 3376, 3304, 3495, 3572, 3672, 2335, 2389, 3167, 2267, 2971, 3218]. **valued** [1698, 1843]. **values** [3238, 2162, 224, 3727, 1960, 419, 508, 3371, 1233, 2428]. **vanadium** [1880]. **vanished** [1745, 1754, 1798, 1871, 2060, 2029, 2118, 2178, 2253, 2392, 2410, 2322, 2544, 2524, 2549, 2472, 2632, 2595, 2673, 2623, 2662, 2691, 2709, 2908, 2734, 2566, 2633, 3242, 3186, 3278, 2507, 2511, 1904, 2098, 2317, 2381, 2370,

2455, 2930, 2648, 3030, 2594]. **vanishing** [3471]. **vapor** [2267]. **vapors** [1208]. **variability** [2307, 2555]. **Variable** [1024, 1208, 1777, 2162, 2168, 3578, 2682, 2831, 2184, 3522, 1504, 1588, 1684, 3435, 3189, 1240, 963, 987]. **variable-step** [963]. **Variables** [1087, 1243, 2329, 1909, 2700, 989]. **variably** [1254]. **variance** [2565]. **variants** [3111]. **variate** [2379]. **variation** [1970, 2162, 1383, 3616, 1968, 1969]. **Variational** [777, 931, 2176, 391, 1736, 511, 415, 2516, 2597, 275, 1156, 3312, 3606, 3065, 648, 1477, 3386, 2346, 2481, 2149, 3088, 3244, 2836, 1386, 2333, 20, 1941, 2302, 2723, 3424]. **variationally** [2130, 2144]. **variety** [2198]. **Various** [3503, 1897, 2638, 2637, 3327, 3376, 989]. **varying** [2438, 1356, 1373, 1276]. **VB** [721, 584]. **Vector** [927, 914, 2731, 2982, 2230, 564, 598, 984, 1370, 1915, 2572, 2782, 2984, 3315, 2878, 1338, 1468, 147, 1244, 1846, 2700, 1801, 3357, 3622, 2883, 2731]. **vectorial** [2892]. **Vectors** [916, 428, 2665, 2984, 3004, 3634, 3296, 1698, 1473]. **vehicles** [2787]. **Velazquez** [3245]. **velocity** [2518]. **Verhulst** [2576]. **verification** [3198]. **Verma** [2877]. **version** [331, 1291, 1297]. **Versus** [846, 3734, 3542, 360, 2596, 2028, 2229]. **Vertex** [2663, 3694, 1591, 208, 260, 408, 273, 305, 3119, 3263, 3326, 1571]. **vertex-angle** [408]. **vertex-decorated** [3326]. **Vertgeim** [2757]. **vertical** [2521]. **Vertices** [1090, 1109, 1120, 294, 612, 360, 2983, 1270, 1424, 1470, 1574, 1575, 3093, 232, 1264]. **very** [3497, 3608]. **vesicles** [101, 347]. **vessel** [987]. **VH** [1438]. **VI** [1170, 442, 770]. **Via** [1160, 3639, 580, 1696, 1697, 1972, 949, 957, 1632, 1735, 1860, 1546, 2343, 2120, 2016, 2043, 2879, 2282, 3696, 2513, 1019, 1156, 3448, 2320, 3171, 1929, 1994, 3567, 2899, 3650, 3740, 2039, 3513, 3421, 2293, 2336, 2639, 3669, 1099, 8, 561, 3093, 164, 2338, 3405, 1670, 1165, 2396, 2204, 2839, 2854, 3042]. **vibrating** [1514, 3590]. **vibration** [1477, 2413]. **vibration-dissociation** [2413]. **Vibrational** [1065, 733, 734, 1478, 329, 367, 3207, 1395, 3512, 532, 2352, 1977, 2224]. **Vibrations** [1068, 1094, 2445, 2710]. **vibron** [2123]. **vibronic** [2264]. **Vieta** [3584]. **view** [2504, 2109, 2188, 3519, 2962, 615]. **viewpoint** [531]. **VII** [443]. **VIII** [271]. **viral** [3642]. **virial** [1994, 2717, 3058, 2931]. **virotherapy** [3098]. **virtual** [3530, 1894, 195]. **virtual-bond** [195]. **virus** [1651, 1975]. **viruses** [2234]. **viscous** [2694, 3573]. **visible** [1711]. **Visualization** [1339, 3036]. **Visualizing** [2773]. **vitro** [3320, 3358, 169, 453, 510]. **vivo** [1085, 2741, 2740, 2702, 3292, 3570, 169, 3288]. **Voigt** [3571]. **vol** [1456]. **Volatilities** [1273]. **voltage** [2860]. **Volterra** [1955, 2337, 645, 640, 115, 1276, 2302]. **Volume** [1187, 1885, 2376, 1040, 3488]. **Volumes** [839, 393, 47]. **volumina** [588]. **volunteer** [1934]. **Voronoi** [2080, 1864]. **vorticity** [2550]. **vs** [3431, 459]. **vulcanization** [1717, 1592, 1841, 2073, 2221, 2489, 2711]. **vulcanized** [2155, 2295].

W [3146]. **Waals** [52, 1315, 2802, 2267, 599]. **wagging** [469]. **wake** [2305]. **wake-free** [2305]. **Wales** [3345]. **walk** [3700, 1404, 2289, 2303].

walk-entropies [3700]. **walks** [3338, 3700, 2825, 264, 1406, 2396, 1402]. **wall** [3185]. **walled** [2070, 3550, 3688]. **Wallis** [379]. **walls** [1406]. **Walsh** [18, 2599]. **Wang** [405]. **warning** [3121]. **washout** [1254, 1340]. **Water** [3206, 1897, 3205, 3500, 3570, 1555, 2646, 3590, 1856, 1935, 2972, 1534, 1551, 1731]. **waterborne** [1550]. **Wave** [1162, 1065, 2669, 1971, 2951, 2016, 2043, 3343, 2923, 1385, 1468, 1604, 2384, 632, 2379, 2039, 2896, 1718, 3151, 3421, 2980, 436, 2690, 2469, 1855, 2989, 1519, 621, 1670, 2630, 2703, 677, 3670, 1829]. **wave-function** [2016, 2043]. **wave-functions** [2384]. **waveform** [3101]. **Wavefunction** [1052, 521, 2033, 2338]. **wavefunctions** [2148, 3520, 286, 3202, 730, 584]. **wavelength** [2873, 3446, 1711]. **wavelength-dependent** [2873]. **Wavelet** [1034, 2085, 3282, 3533, 3398, 1322, 1358, 2464, 3361, 1751, 2245, 2248, 648, 3262, 2244, 2583, 3008, 3633, 3513, 2529, 1501, 3669, 2558, 2333, 2405, 3297, 3584, 3266, 3611, 3704, 2241, 1520]. **Wavelet-based** [3533, 1358, 2245, 3008]. **wavelet-distributed** [648]. **wavelet-finite** [2529]. **Wavelets** [567, 3054, 3215, 3011, 1758, 2626]. **Waves** [816, 874, 907, 3576, 550, 955, 1035, 1383, 2045, 2744, 410, 450, 1403, 2305, 518, 11, 497, 2806, 2582]. **Way** [921, 638, 2701, 471, 2415, 3485, 2423]. **ways** [2238]. **Weak** [2183, 1743, 1920, 2904, 378, 3705, 525]. **weak-branching** [525]. **Weaker** [3108]. **Weakly** [3535, 3342, 1896, 2973, 2575, 2925, 3595, 2351, 3467]. **Weber** [875, 1004]. **Wegscheider** [51]. **Wei** [2275]. **Weight** [2563, 2591, 1553, 1724, 2399, 1879]. **Weighted** [2386, 1070, 2707, 441, 442, 443, 1753, 3025, 98, 237, 2080, 3326, 2650]. **weighted-shifted** [3025]. **weighting** [394]. **weights** [614, 584, 3622]. **Weiming** [1297]. **Weizsäcker** [1868, 2187]. **welcome** [2]. **Well** [1065, 1982, 2016, 2043, 2101, 1906, 2214, 2439, 3469, 3333, 2530, 482, 560, 622, 1803]. **wetted** [1531]. **Weyl** [1131, 1009]. **Wheland** [358]. **where** [3492]. **Which** [905, 1858]. **white** [3405, 2616]. **Whittaker** [3120]. **whole** [1193]. **whose** [612, 2207]. **Wick** [2418]. **Wick-type** [2418]. **wide** [2732]. **widths** [2842, 2216]. **Wiener** [2871, 66, 122, 224, 180, 1146, 1517, 3482, 847, 1581, 39, 3733, 2613, 1222, 2966, 1058, 1209, 1589]. **Wigner** [1486, 485, 613, 1290]. **Willard** [2230]. **Windows** [2369]. **wine** [1537]. **wire** [2750]. **with-** [3028]. **within** [743, 2111, 3590, 3387, 2186, 719, 2115, 3723, 189, 2660, 2536, 2192, 2787, 584, 1278]. **Without** [1075, 1150, 3648, 3500, 3570, 3735, 990, 3392, 1040, 3216, 2040, 2588, 2379, 1450, 30, 3028]. **Witten** [2132]. **WKB** [877]. **Wong** [3405]. **Woodbury** [3149]. **Woods** [1280]. **word** [1307]. **wordlengths** [277]. **work** [70]. **workout** [2983]. **world** [3693]. **wreath** [2696]. **Wright** [2952]. **writhe** [2629]. **writing** [456]. **WTMEMPR** [2707].

X [3641, 953, 1296, 1260, 1442, 2968, 3688, 3641, 2337, 3096, 683, 3220]. **X-graphene** [3688]. **X-ray** [2337, 3096]. **X-trees** [3220]. **XBCD** [501, 502]. **Xe** [1096, 250]. **XXI** [4]. **XXII** [5]. **XXIV** [22]. **XY** [1393, 2435].

Y-graphene [3688]. **Y-junctions** [3515]. **Y.-H** [2872]. **YAG**

[3307, 972, 1509, 2055]. **Yamanouchi** [697]. **YBa** [498]. **years** [623, 312]. **Yield** [1024, 2651, 2510, 2168, 1504, 1240, 987]. **Yielding** [807]. **Yields** [1022, 1007, 1053, 1498]. **Yorke** [2228, 1997]. **Yttrium** [1152, 3307]. **Yukawa** [415, 275, 1050, 1659, 1769, 3267, 3394].

z [1483]. **zag** [2768]. **Zagreb** [1516, 1706, 2889, 1439, 3038, 1177, 2977, 1730]. **Zakai** [3405]. **Zakharov** [3189]. **Zeeman** [661, 2992]. **Zeldovich** [1818]. **Zeolite** [1074, 1010, 173]. **Zeolite-like** [1010]. **Zero** [792, 801, 2748, 1328, 793, 2749, 1559, 3286, 329, 3277, 1905, 1840, 2628, 2505, 2717, 3172, 3243, 3045, 3261, 2840, 677, 3160, 3218]. **zero-point** [329]. **zero-pressure** [2717]. **zero-range** [677]. **zeros** [2741]. **Zeroth** [1121, 1176, 1265, 1771]. **Zeroth-order** [1121, 1176, 1265, 1771]. **Zeta** [2526, 2586, 3481]. **Zhabotinskii** [2313, 2658, 1690, 1679, 377, 151, 410, 2228, 2177, 2199, 2559, 2628, 2615, 3140, 2505, 1997, 2065]. **Zhabotinsky** [3226, 2937, 858]. **Zhang** [1978, 1507]. **ZIBgridfree** [2314]. **zig** [2768]. **zig-zag** [2768]. **zigzag** [3647, 3734, 2863, 994]. **zigzagging** [1146]. **Ziv** [1702, 1563]. **Zn** [3641, 1513]. **Zubov** [1013]. **Zubov-like** [1013]. **zymogen** [1723, 1724].

References

Rouvray:1987:EFa

[1] Dennis H. Rouvray. Editorial foreword. *Journal of Mathematical Chemistry*, 1(1):iii–iv, March 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01205333; http://link.springer.com/article/10.1007/BF01205333`.

Anonymous:1987:LW

[2] Anonymous. Letters of welcome. *Journal of Mathematical Chemistry*, 1(1):v–vii, March 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01205334; http://link.springer.com/article/10.1007/BF01205334`.

Sumners:1987:KTM

[3] D. W. Sumners. The knot theory of molecules. *Journal of Mathematical Chemistry*, 1(1):1–14, March 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205335`.

King:1987:CATa

[4] R. B. King. Chemical applications of topology and group theory. XXI: Chirality in transitive skeletons and qualitative completeness [1]. *Jour-*

nal of Mathematical Chemistry, 1(1):15–44, March 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205336`.

King:1987:CATb

[5] R. B. King. Chemical applications of topology and group theory. XXII: Lowest degree chirality polynomials for regular polyhedra [1]. *Journal of Mathematical Chemistry*, 1(1):45–59, March 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205337`.

Filip:1987:NAD

[6] P. A. Filip, T.-S. Balaban, and A. T. Balaban. A new approach for devising local graph invariants: Derived topological indices with low degeneracy and good correlation ability. *Journal of Mathematical Chemistry*, 1(1):61–83, March 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205338`.

Otto:1987:CRE

[7] P. Otto, J. Ladik, and P. G. Mezey. A convexity relation for the energies of certain polymers of unit cells of different sizes. *Journal of Mathematical Chemistry*, 1(1):85–96, March 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205339`.

Randic:1987:ECP

[8] Milan Randić. On the evaluation of the characteristic polynomial via symmetric function theory. *Journal of Mathematical Chemistry*, 1(1):145–152, March 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205340`.

El-Basil:1987:ACT

[9] Sherif El-Basil. Applications of caterpillar trees in chemistry and physics. *Journal of Mathematical Chemistry*, 1(2):153–174, July 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205666`.

Kirby:1987:FCG

[10] E. C. Kirby. The factorisation of chemical graphs and their polynomials: A systematic study of certain trees. *Journal of Mathematical Chemistry*, 1(2):175–218, July 1987. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205667`.

Schneider:1987:QAM

[11] K. R. Schneider, B. Wegner, and J. Tóth. Qualitative analysis of a model for synaptic slow waves. *Journal of Mathematical Chemistry*, 1 (2):219–234, July 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205668`.

Edward:1987:MAB

[12] R. Birnbaum Edward and A. Walker Elbert. A mathematical analysis of the Bjerrum function for the stepwise equilibrium model. *Journal of Mathematical Chemistry*, 1(2):235–247, July 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205669`.

King:1987:DTC

[13] R. Bruce King. The dimensionality and topology of chemical bonding manifolds in metal clusters and related compounds. *Journal of Mathematical Chemistry*, 1(3):249–265, September 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01179793`.

Fernandez:1987:CPP

[14] Francisco M. Fernández, Gustavo A. Arteca, and Eduardo A. Castro. Critical parameters from power series expansions. *Journal of Mathematical Chemistry*, 1(3):267–280, September 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01179794`.

El-Basil:1987:GLP

[15] S. El-Basil and M. Randić. On global and local properties of Clar pi-electron sextets. *Journal of Mathematical Chemistry*, 1(3):281–307, September 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01179795`.

Klein:1987:RRN

[16] D. J. Klein, T. P. Zivković, and N. Trinajstić. Resonance in random π-network polymers. *Journal of Mathematical Chemistry*, 1(3):309–334, September 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01179796`.

Rouvray:1987:EFb

[17] Dennis H. Rouvray. Editorial foreword. *Journal of Mathematical Chemistry*, 1(4):i, November 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01205065; http://link.springer.com/article/10.1007/BF01205065`.

OLeary:1987:WDH

[18] Brian O'Leary and R. B. Mallion. Walsh diagrams and the Hellmann–Feynman theorem: A tribute to the late Professor Charles A. Coulson, F.R.S. (1910–1974). *Journal of Mathematical Chemistry*, 1(4): 335–344, November 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205066`.

Bonchev:1987:CIL

[19] D. Bonchev, D. Kamenski, and O. N. Temkin. Complexity index for the linear mechanisms of chemical reactions. *Journal of Mathematical Chemistry*, 1(4):345–388, November 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205067`.

Scholberg:1987:EBP

[20] Harold M. Scholberg. An examination of the basic postulates of surface chemistry: A variational calculus analysis of the classic rotating drop experiment. *Journal of Mathematical Chemistry*, 1(4):389–403, November 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205068`.

Berman:1987:HPC

[21] D. M. Berman and K. W. Holladay. Homomorphism polynomials of chemical graphs. *Journal of Mathematical Chemistry*, 1(4):405–414, November 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205069`.

King:1987:CATc

[22] R. Bruce King. Chemical applications of topology and group theory. XXIV: Chiralization of chemically significant polyhedra [1]. *Journal of Mathematical Chemistry*, 1(4):415–421, November 1987. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01205070`.

Rouvray:1988:EFa

[23] Dennis H. Rouvray. Editorial foreword. *Journal of Mathematical Chemistry*, 2(1):vii, February 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01166465; http://link.springer.com/article/10.1007/BF01166465`.

El-Basil:1988:TCA

[24] S. El-Basil. Theory and computational applications of Fibonacci graphs. *Journal of Mathematical Chemistry*, 2(1):1–29, February 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166466`.

Bangov:1988:CAS

[25] I. P. Bangov and K. D. Kanev. Computer-assisted structure generation from a gross formula: II. Multiple bond unsaturated and cyclic compounds. Employment of fragments. *Journal of Mathematical Chemistry*, 2(1):31–48, February 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166467`.

Mcquistan:1988:SOM

[26] R. B. Mcquistan and J. L. Hock. The shift operator matrix method applied to the two-dimensional nearest and next nearest neighbor problem. *Journal of Mathematical Chemistry*, 2(1):49–68, February 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166468`.

Balasubramanian:1988:TPL

[27] K. Balasubramanian. Tree pruning and lattice statistics on Bethe lattices. *Journal of Mathematical Chemistry*, 2(1):69–82, February 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166469`.

Kirby:1988:NSC

[28] E. C. Kirby. A note on some coefficients of the Chebyshev polynomial form of the characteristic polynomial. *Journal of Mathematical Chemistry*, 2(1):83–87, February 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166470`.

King:1988:CP

[29] R. Bruce King. Chirality polynomials. *Journal of Mathematical Chemistry*, 2(2):89–115, April 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165923`.

Sinanoglu:1988:NPSa

[30] Oktay Sinanoglu. The new pictorial structural covariance method for qualitative quantum chemistry. II: Arenes with or without polyene side chains and polyene bridges. *Journal of Mathematical Chemistry*, 2(2): 117–136, April 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165924`.

Sinanoglu:1988:NPSb

[31] Oktay Sinanoglu. The new pictorial structural covariance method for qualitative quantum chemistry. III: Fused polycyclics and their ions. *Journal of Mathematical Chemistry*, 2(2):137–154, April 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165925`.

Herndon:1988:LNB

[32] W. C. Herndon and A. J. Bruce. Linear notation for benzenoid aromatic hydrocarbons. Molecular similarity based on notation similarity. *Journal of Mathematical Chemistry*, 2(2):155–169, April 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165926`.

Mikulecky:1988:RRS

[33] D. C. Mikulecky and F. Sauer. The role of the reference state in nonlinear kinetic models: Network thermodynamics leads to a linear and reciprocal coordinate system far from equilibrium. *Journal of Mathematical Chemistry*, 2(2):171–196, April 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165927`.

Trinajstic:1988:CPC

[34] Nenad Trinajstić. The characteristic polynomial of a chemical graph. *Journal of Mathematical Chemistry*, 2(3):197–215, July 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01167201`.

Villaveces:1988:APE

[35] J. L. C. Villaveces, C. G. A. Arteca, F. M. Fernández, and E. A. Castro. Approximate polynomial expressions for Rydberg–Klein–Rees curves of diatomic covalent molecules. *Journal of Mathematical Chemistry*, 2 (3):217–226, July 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01167202`.

Arteca:1988:NMC

[36] Gustavo A. Arteca, Francisco M. Fernández, and Eduardo A. Castro. New method for confluent singularity analysis of power series. *Journal of Mathematical Chemistry*, 2(3):227–239, July 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01167203`.

Battaglia:1988:PTT

[37] F. Battaglia and F. George. A Pascal type triangle for the number of topologically distinct many-electron Feynman graphs. *Journal of Mathematical Chemistry*, 2(3):241–247, July 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01167204`.

Randic:1988:IM

[38] M. Randić and B. Baker. Isospectral multitrees. *Journal of Mathematical Chemistry*, 2(3):249–265, July 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01167205`.

Mohar:1988:HCW

[39] Bojan Mohar and Tomaz Pisanski. How to compute the Wiener index of a graph. *Journal of Mathematical Chemistry*, 2(3):267–277, July 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01167206`.

Mukherjee:1988:ELE

[40] Asok K. Mukherjee. Eigenvalues of large even annulenes in terms of K_3, S_4 and S_5. *Journal of Mathematical Chemistry*, 2(3):279–286, July 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01167207`.

Bodroza:1988:NKS

[41] O. Bodroza, I. Gutman, S. J. Cyvin, and R. Tosić. Number of Kekulé structures of hexagon-shaped benzenoids. *Journal of Mathematical*

Chemistry, 2(3):287–298, July 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01167208`.

Rouvray:1988:EFb

[42] Dennis H. Rouvray. Editorial foreword. *Journal of Mathematical Chemistry*, 2(4):i, October 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01166297; http://link.springer.com/article/10.1007/BF01166297`.

Mezey:1988:SGS

[43] Paul G. Mezey. Shape group studies of molecular similarity: Shape groups and shape graphs of molecular contour surfaces. *Journal of Mathematical Chemistry*, 2(4):299–323, October 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166298`.

Mezey:1988:GLR

[44] Paul G. Mezey. Global and local relative convexity and oriented relative convexity; application to molecular shapes in external fields. *Journal of Mathematical Chemistry*, 2(4):325–346, October 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166299`.

Mekenyan:1988:TIM

[45] Ovanes Mekenyan, Danail Bonchev, and Alexandru Balaban. Topological indices for molecular fragments and new graph invariants. *Journal of Mathematical Chemistry*, 2(4):347–375, October 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166300`.

Harary:1988:GSS

[46] Frank Harary and Pad G. Mezey. Graphical shapes: Seeing graphs of chemical curves and molecular surfaces. *Journal of Mathematical Chemistry*, 2(4):377–389, October 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166301`.

Radhakrishnan:1988:MVA

[47] T. P. Radhakrishnan and W. C. Herndon. Molar volumes of alkanes and topological indices. *Journal of Mathematical Chemistry*, 2(4):391–399, October 1988. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166302.

Turanyi:1988:MQS

[48] T. Turanyi, T. Berces, and J. Tóth. The method of quasi-stationary sensitivity analysis. *Journal of Mathematical Chemistry*, 2(4):401–409, October 1988. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166303.

Rouvray:1989:EFa

[49] Dennis H. Rouvray. Editorial foreword. *Journal of Mathematical Chemistry*, 3(1):vi, January 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/BF01171881; http://link.springer.com/article/10.1007/BF01171881.

El-Basil:1989:FNT

[50] Sherif El-Basil and Douglas J. Klein. Fibonacci numbers in the topological theory of benzenoid hydrocarbons and related graphs. *Journal of Mathematical Chemistry*, 3(1):1–23, January 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01171882.

Schuster:1989:GWC

[51] Stefan Schuster and Ronny Schuster. A generalization of Wegscheider's condition. Implications for properties of steady states and for quasi-steady-state approximation. *Journal of Mathematical Chemistry*, 3(1):25–42, January 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01171883.

Arteca:1989:SGT

[52] Gustavo A. Arteca and Paul G. Mezey. Shape group theory of van der Waals surfaces. *Journal of Mathematical Chemistry*, 3(1):43–71, January 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01171884.

Koca:1989:MMRa

[53] Jaroslav Koca. A mathematical model of realistic constitutional chemistry. A synthon approach. I: An algebraic model of a synthon. *Journal*

of Mathematical Chemistry, 3(1):73–89, January 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01171885.

Koca:1989:MMRb

[54] Jaroslav Koca. A mathematical model of realistic constitutional chemistry. A synthon approach. II: The model and organic synthesis. *Journal of Mathematical Chemistry*, 3(1):91–115, January 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01171886.

Rouvray:1989:EFb

[55] Dennis H. Rouvray. Editorial foreword. *Journal of Mathematical Chemistry*, 3(2):i, April 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/BF01166044; http://link.springer.com/article/10.1007/BF01166044.

Johnson:1989:REM

[56] M. A. Johnson. A review and examination of the mathematical spaces underlying molecular similarity analysis. *Journal of Mathematical Chemistry*, 3(2):117–145, April 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166045.

Balasubramanian:1989:CPS

[57] K. Balasubramanian. Characteristic polynomials of spirographs. *Journal of Mathematical Chemistry*, 3(2):147–159, April 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166046.

Kvasnick:1989:TMG

[58] V. Kvasničk and A. J. Pospíchal. Two metrics for a graph-theoretical model of organic chemistry. *Journal of Mathematical Chemistry*, 3(2):161–191, April 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166047.

Poshusta:1989:EFT

[59] R. D. Poshusta and M. C. McHughes. Embedding frequencies of trees. *Journal of Mathematical Chemistry*, 3(2):193–215, April 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166048.

Gupta:1989:SOP

[60] A. K. Das Gupta and C. Dutta. Symmetry and other properties of second-order phenomenological coefficients and their significance in a chemical system. *Journal of Mathematical Chemistry*, 3 (2):217–226, April 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166049`.

Balasubramanian:1989:RCI

[61] K. Balasubramanian. Reduced cycle indices and their applications in enumeration of NMR signals and equivalence classes. *Journal of Mathematical Chemistry*, 3(2):227–232, April 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166050`.

Rouvray:1989:EFc

[62] Dennis H. Rouvray. Editorial foreword. *Journal of Mathematical Chemistry*, 3(3):i, July 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01169593; http://link.springer.com/article/10.1007/BF01169593`.

Hall:1989:RPH

[63] G. G. Hall and J. R. Dias. The recognition of polyrex hydrocarbon radicals. *Journal of Mathematical Chemistry*, 3(3):233–242, July 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169594`.

Wulfman:1989:GSAa

[64] C. E. Wulfman and H. Rabitz. Global sensitivity analysis of nonlinear chemical kinetic equations using Lie groups: I. Determination of one-parameter groups. *Journal of Mathematical Chemistry*, 3(3): 243–259, July 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169595`.

Wulfman:1989:GSAb

[65] C. E. Wulfman and H. Rabitz. Global sensitivity analysis of nonlinear chemical kinetic equations using Lie groups: II. Some chemical and mathematical properties of the transformation groups. *Journal of Mathematical Chemistry*, 3(3):261–297, July 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169596`.

Bogdanov:1989:TDW

[66] B. Bogdanov, S. Nikolić, and N. Trinajstić. On the three-dimensional Wiener number. *Journal of Mathematical Chemistry*, 3(3):299–309, July 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169597`. See comment [122].

Tosi:1989:ILE

[67] C. Tosi, R. Fusco, L. Caccianotti, and V. Parisi. On the investigation of the low-energy conformational space of molecules. *Journal of Mathematical Chemistry*, 3(3):311–320, July 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169598`.

Mezey:1989:OPMa

[68] P. G. Mezey. Open problems in mathematical chemistry. *Journal of Mathematical Chemistry*, 3(3):321, July 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01169599; http://link.springer.com/article/10.1007/BF01169599`.

Rouvray:1989:EFd

[69] Dennis H. Rouvray. Editorial foreword. *Journal of Mathematical Chemistry*, 3(4):i–ii, December 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01169014; http://link.springer.com/article/10.1007/BF01169014`.

OLeary:1989:CCW

[70] Brian O'Leary and R. B. Mallion. C. A. Coulson's work on a contour-integral approach to the London theory of magnetic susceptibility of conjugated molecules. *Journal of Mathematical Chemistry*, 3(4):323–342, December 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169015`.

Gutman:1989:FDD

[71] I. Gutman. Factors determining the direction of the stereoselection process in the generalized Frank model. *Journal of Mathematical Chemistry*, 3(4):343–355, December 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169016`.

Jiang:1989:MCP

[72] Y. Jiang and H. Zhang. Moments and characteristic polynomials of bipartite Hückel graphs. *Journal of Mathematical Chemistry*, 3(4):357–375, December 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169017`.

Sakurai:1989:PRP

[73] K. Sakurai and K. Nishimoto. Propagator representation for partial structure character in conjugated systems. *Journal of Mathematical Chemistry*, 3(4):377–382, December 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169018`.

Narumi:1989:PGE

[74] Hideyuki Narumi and Haruo Hosoya. Proof of the generalized expressions for the number of perfect matchings of polycube graphs. *Journal of Mathematical Chemistry*, 3(4):383–391, December 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169019`.

Tosic:1989:EKS

[75] R. Tosić and S. J. Cyvin. Enumeration of Kekulé structures in benzenoid hydrocarbons: "flounders". *Journal of Mathematical Chemistry*, 3(4):393–401, December 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169020`.

Mohar:1989:CCP

[76] Bojan Mohar. Computing the characteristic polynomial of a tree. *Journal of Mathematical Chemistry*, 3(4):403–406, December 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169021`.

Mezey:1989:OPMb

[77] P. G. Mezey. Open problems in mathematical chemistry. *Journal of Mathematical Chemistry*, 3(4):407, December 1989. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01169022; http://link.springer.com/article/10.1007/BF01169022`.

Rouvray:1990:EF

[78] Dennis H. Rouvray. Editorial foreword. *Journal of Mathematical Chemistry*, 4(1):vii–viii, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01169999; http://link.springer.com/article/10.1007/BF01169999`.

Lowdin:1990:MCM

[79] Per-Olov Löwdin. Mathematics in chemistry and in mathematical chemistry. *Journal of Mathematical Chemistry*, 4(1):3–14, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170000`. Proc. Galveston Conference on Mathematical Chemistry. Accepted for publication.

Dias:1990:FPT

[80] Jerry Ray Dias. A formula periodic table for benzenoid hydrocarbons and the Aufbau and excised internal structure concepts in benzenoid enumerations. *Journal of Mathematical Chemistry*, 4(1):17–29, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170001`.

Kirby:1990:HPP

[81] E. C. Kirby. Hamiltonian paths in polyhexes: The use of branching subgraphs to assist diagnosis of graph traceability. *Journal of Mathematical Chemistry*, 4(1):31–46, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170002`.

Cyvin:1990:HCN

[82] S. J. Cyvin, J. Brunvoll, and B. N. Cyvin. The hunt for concealed non–Kekuléan polyhexes. *Journal of Mathematical Chemistry*, 4(1):47–54, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170003`.

Elk:1990:COP

[83] Seymour B. Elk. A canonical ordering of polybenzenes and polymantanes using a prime number factorization technique. *Journal of Mathematical Chemistry*, 4(1):55–68, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170004`.

King:1990:TDA

[84] R. B. King. Three-dimensional aromaticity: A topological analysis of computational methods. *Journal of Mathematical Chemistry*, 4(1): 69–85, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170005`.

Balasubramanian:1990:RDT

[85] K. Balasubramanian. Recent developments in tree-pruning methods and polynomials for cactus graphs and trees. *Journal of Mathematical Chemistry*, 4(1):89–102, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170006`.

Jiang:1990:SAM

[86] Yuansheng Jiang and Guangyao Chen. On subspectral acyclic molecular graphs. *Journal of Mathematical Chemistry*, 4(1):103–115, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170007`.

Ellzey:1990:ECD

[87] M. L. Ellzey, Jr. Eigenvalue correlation diagrams for effective Hamiltonians: The ESR spectrum of axial Gd(III). *Journal of Mathematical Chemistry*, 4(1):117–126, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170008`.

Dias:1990:TSH

[88] Jerry Ray Dias. A theoretical study of π-hydrocarbon-iron tricarbonyl complexes. *Journal of Mathematical Chemistry*, 4(1):127–142, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170009`.

Zivkovic:1990:SPE

[89] T. P. Zivković. Solution of the perturbed eigenvalue equation by the low-rank perturbation method. *Journal of Mathematical Chemistry*, 4(1): 143–153, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170010`.

Randic:1990:NCS

[90] Milan Randić. The nature of chemical structure. *Journal of Mathematical Chemistry*, 4(1):157–184, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170011`.

Basak:1990:OCS

[91] Subhash C. Basak, Gerald J. Niemi, and Gilman D. Veith. Optimal characterization of structure for prediction of properties. *Journal of Mathematical Chemistry*, 4(1):185–205, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170012`.

Mekenyan:1990:OCP

[92] O. Mekenyan, S. Karabunarlev, and D. Bonchev. The OASIS concept for predicting the biological activity of chemical compounds. *Journal of Mathematical Chemistry*, 4(1):207–215, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170013`.

Jerman-Blazic:1990:SMS

[93] Borka Jerman-Blazic and Milan Randić. Similarity measures for sets of strings and application in chemical classification. *Journal of Mathematical Chemistry*, 4(1):217–225, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170014`.

McHughes:1990:GTC

[94] Mary C. McHughes and R. D. Poshusta. Graph-theoretic cluster expansions. Thermochemical properties for alkanes. *Journal of Mathematical Chemistry*, 4(1):227–249, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170015`.

Matsen:1990:FEP

[95] F. A. Matsen. The freeon N-electron procedure and the Hubbard connection. *Journal of Mathematical Chemistry*, 4(1):253–269, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170016`.

March:1990:SCE

[96] N. H. March. Strongly correlated electronic ground states in metals near the metal-insulator transition. *Journal of Mathematical Chemistry*, 4(1):

271–293, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170017`.

Li:1990:UGT

[97] Xiangzhu Li and Josef Paldus. Unitary group tensor operator algebras for many-electron systems: I. Clebsch–Gordan and Racah coefficients. *Journal of Mathematical Chemistry*, 4(1):295–353, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170018`.

Nikolic:1990:CWS

[98] Sonja Nikolić, Nenad Trinajstić, Jan V. Knop, Wolfgang R. Müller, and Klaus Szymanski. On the concept of the weighted spanning tree of dualist. *Journal of Mathematical Chemistry*, 4(1):357–375, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170019`.

Mezey:1990:PSG

[99] Paul G. Mezey. Point symmetry groups of all distorted configurations of a molecule form a lattice. *Journal of Mathematical Chemistry*, 4(1):377–381, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170020`.

Darsey:1990:HOM

[100] Jerry A. Darsey and Wayne L. Mattice. A harmonic oscillator model of the conformationally flexible helical polymeric molecules. *Journal of Mathematical Chemistry*, 4(1):383–394, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170021`.

Fisher:1990:SMT

[101] Michael E. Fisher. The statistical mechanics of two-dimensional vesicles. *Journal of Mathematical Chemistry*, 4(1):395–399, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01170022`.

Lowdin:1990:CCM

[102] Per-Olov Löwdin. Concepts of convergence in mathematical chemistry. *Journal of Mathematical Chemistry*, 4(1):401–414, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.`

1007/BF01170023. Proc. Galveston Conference on Mathematical Chemistry. Accepted for publication.

Mallion:1990:GJC

[103] R. B. Mallion and D. H. Rouvray. The golden jubilee of the Coulson–Rushbrooke pairing theorem. *Journal of Mathematical Chemistry*, 5 (1):1–21, March 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166272. See postscript [209].

Ohkami:1990:GTA

[104] Noriko Ohkami. Graph-theoretical analysis of the sextet polynomial. Proof of the correspondence between the sextet patterns and Kekulé patterns. *Journal of Mathematical Chemistry*, 5(1):23–42, March 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166273.

Bonchev:1990:CGM

[105] D. Bonchev, V. Kamenska, and O. Mekenyan. Comparability graphs and molecular properties: IV. Generalizations and applications. *Journal of Mathematical Chemistry*, 5(1):43–72, March 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166274.

Zhixing:1990:FET

[106] Chen Zhixing. Free-electron theory of substituent effects on molecular orbital coefficients. *Journal of Mathematical Chemistry*, 5(1): 73–79, March 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166275.

Gutman:1990:PCC

[107] Ivan Gutman and Noriyuki Mizoguchi. A property of the circuit characteristic polynomial. *Journal of Mathematical Chemistry*, 5(1):81–82, March 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/BF01166276; http://link.springer.com/article/10.1007/BF01166276.

Lee:1990:FCP

[108] M. Howard Lee. Fermionic chemical potential. *Journal of Mathematical Chemistry*, 5(2):83–98, June 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166422.

Fujita:1990:ECS

[109] Shinsaku Fujita. Enumerations of chemical structures by subduction of coset representations. Correlation of unit subduced cycle indices to Pólya's cycle indices. *Journal of Mathematical Chemistry*, 5 (2):99–120, June 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166423`.

Fujita:1990:SCR

[110] Shinsaku Fujita. Subduction of coset representations. An application to enumeration of chemical structures with achiral and chiral ligands. *Journal of Mathematical Chemistry*, 5(2):121–156, June 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166424`.

Xiaofeng:1990:RKB

[111] Guo Xiaofeng and Zhang Fuji. Recognizing Kekuléan benzenoid systems by C–P–V path elimination. *Journal of Mathematical Chemistry*, 5(2):157–170, June 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166425`.

Trinajstic:1990:CPH

[112] Nenad Trinajstić. On the classification of polyhex hydrocarbons. *Journal of Mathematical Chemistry*, 5(2):171–175, June 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166426`.

Estrin:1990:PEC

[113] D. A. Estrín, F. M. Fernández, and E. A. Castro. Potential energy curves of diatomic molecules from the Hill determinant method. *Journal of Mathematical Chemistry*, 5(2):177–185, June 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166427`.

Bhalekar:1990:GPI

[114] Anil A. Bhalekar. On the generalized phenomenological irreversible thermodynamic theory (GPITT). *Journal of Mathematical Chemistry*, 5 (2):187–196, June 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166428`.

Hering:1990:OLV

[115] Roger H. Hering. Oscillations in Lotka–Volterra systems of chemical reactions. *Journal of Mathematical Chemistry*, 5(2):197–202, June 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166429`.

Turanyi:1990:SAC

[116] Tamás Turányi. Sensitivity analysis of complex kinetic systems. Tools and applications. *Journal of Mathematical Chemistry*, 5(3):203–248, September 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166355`.

Hamilton:1990:EIE

[117] G. R. Hamilton, W. G. Laidlaw, R. Maier, and R. B. Flewwelling. The effect of inhomogeneities on evaluation of a fractal dimension for objects on a lattice. *Journal of Mathematical Chemistry*, 5(3):249–263, September 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166356`.

Gornick:1990:RAS

[118] Fred Gornick and Richard W. Freedman. Reactions of adjacent substituents on polymer chains: Combinatorial consequences of the mechanism. *Journal of Mathematical Chemistry*, 5(3):265–274, September 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166357`.

Lowe:1990:IPE

[119] John P. Lowe and Matthew W. Davis. Isospectral points and edges in graph theory. *Journal of Mathematical Chemistry*, 5(3):275–285, September 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166358`.

Huang:1990:LCC

[120] Xun-Cheng Huang. Limit cycles in a continuous fermentation model. *Journal of Mathematical Chemistry*, 5(3):287–296, September 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166359`.

DelRe:1990:SOE

[121] Giuseppe Del Re and Christoph-M. Liegener. Second-order expression of Born probabilities by partitioning and Laplace transform methods. *Journal of Mathematical Chemistry*, 5(3):297–304, September 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166360`.

Bogdanov:1990:TDW

[122] B. Bogdanov, S. Nikolić, and N. Trinajstić. On the three-dimensional Wiener number. A comment. *Journal of Mathematical Chemistry*, 5(3): 305–306, September 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01166361; http://link.springer.com/article/10.1007/BF01166361`. See [66].

Soteros:1990:SPN

[123] Christine E. Soteros and Stuart G. Whittington. Some properties of the numbers of lattice animals and lattice trees. *Journal of Mathematical Chemistry*, 5(3):307–308, September 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01166362; http://link.springer.com/article/10.1007/BF01166362`.

Kvasnicka:1990:GTI

[124] V. Kvasnička and J. Pospíchal. Graph-theoretical interpretation of Ugi's concept of the reaction network. *Journal of Mathematical Chemistry*, 5(4):309–322, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164854`.

Manning:1990:TPP

[125] R. S. Manning and N. De Leon. Theory of projected probabilities on nonorthogonal states: Application to electronic populations in molecules. *Journal of Mathematical Chemistry*, 5(4):323–357, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164855`.

Gimarc:1990:DRG

[126] Benjamin M. Gimarc and Jane J. Ott. Details of the reaction graphs for intramolecular isomerizations of the carboranes. *Journal of Mathematical Chemistry*, 5(4):359–380, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164856`.

Radhakrishnan:1990:EFP

[127] T. P. Radhakrishnan. Euler's formula and phase rule. *Journal of Mathematical Chemistry*, 5(4):381–387, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164857`.

Klopman:1990:EQS

[128] Gilles Klopman and István Kolossváry. Evaluation of quantitative structure-activity predictions. Comparison of the predictive power of an artificial intelligence system with human experts. *Journal of Mathematical Chemistry*, 5(4):389–407, December 1990. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164858`.

Mezey:1991:EFa

[129] Paul G. Mezey and Nenad Trinajstić. Editorial foreword. *Journal of Mathematical Chemistry*, 6(1):v–vi, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01192569; http://link.springer.com/article/10.1007/BF01192569`.

Amann:1991:CSR

[130] Anton Amann. Chirality: A superselection rule generated by the molecular environment? *Journal of Mathematical Chemistry*, 6(1):1–15, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192570`.

Schuster:1991:DSD

[131] Stefan Schuster and Ronny Schuster. Detecting strictly detailed balanced subnetworks in open chemical reaction networks. *Journal of Mathematical Chemistry*, 6(1):17–40, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192571`.

Gutman:1991:GCF

[132] I. Gutman and D. J. Klein. Generalization of Cyvin's formula. *Journal of Mathematical Chemistry*, 6(1):41–50, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192572`.

Ugalde:1991:EEE

[133] Jesus M. Ugalde, C. Sarasola, L. Domínguez, and Russell J. Bovd. The evaluation of electronic extracule and intracule densities and related probability functions in terms of Gaussian basis functions. *Journal of Mathematical Chemistry*, 6(1):51–61, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192573`.

Kvasnicka:1991:ANN

[134] V. Kvasnička. An application of neural networks in chemistry. Prediction of ^{13}C NMR chemical shifts. *Journal of Mathematical Chemistry*, 6(1): 63–76, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192574`.

Dachsel:1991:ACC

[135] Holger Dachsel and Wolfgang Quapp. An analytical computation of Christoffel symbols for reaction coordinate and trajectory treatments under internal coordinates. *Journal of Mathematical Chemistry*, 6(1): 77–90, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192575`.

Seetharamulu:1991:PFP

[136] P. Seetharamulu and Gordon M. Crippen. A potential function for protein folding. *Journal of Mathematical Chemistry*, 6(1):91–110, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192576`.

Cioslowski:1991:CBG

[137] J. Cioslowski. A conjecture on benzenoid graphs. *Journal of Mathematical Chemistry*, 6(1):111, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01192577; http://link.springer.com/article/10.1007/BF01192577`.

Kapral:1991:DMC

[138] Raymond Kapral. Discrete models for chemically reacting systems. *Journal of Mathematical Chemistry*, 6(1):113–163, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192578`.

Demiralp:1991:FCEa

[139] Metin Demiralp and Herschel Rabitz. Factorization of certain evolution operators using Lie algebra: Formulation of the method. *Journal of Mathematical Chemistry*, 6(1):165–191, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192579`.

Demiralp:1991:FCEb

[140] Metin Demiralp and Herschel Rabitz. Factorization of certain evolution operators using Lie algebra: Convergence theorems. *Journal of Mathematical Chemistry*, 6(1):193–204, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192580`.

Arteca:1991:CCE

[141] G. A. Arteca and P. G. Mezey. A conjecture on the change of electronic density of a molecule under an isotropic dilatation of the nuclear geometry. *Journal of Mathematical Chemistry*, 6(1):205–206, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01192581; http://link.springer.com/article/10.1007/BF01192581`.

Broeckhove:1991:GCA

[142] J. Broeckhove, L. Lathouwers, and P. Van Leuven. The generator coordinate approximation for molecules: A review. *Journal of Mathematical Chemistry*, 6(1):207–241, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192582`.

Buda:1991:GCP

[143] Andrzej B. Buda, Thomas P. E. Auf der Heyde, and Kurt Mislow. Geometric chirality products. *Journal of Mathematical Chemistry*, 6(1):243–253, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192583`.

AufderHeyde:1991:DDC

[144] Thomas P. E. Auf der Heyde, Andrzej B. Buda, and Kurt Mislow. Desymmetrization and degree of chirality. *Journal of Mathematical Chemistry*, 6(1):255–265, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192584`.

Brinkmann:1991:AEM

[145] Klaus Brinkmann and Heinz Kleindienst. Analytic evaluation of multicenter integrals for Gaussian-type orbitals. *Journal of Mathematical Chemistry*, 6(1):267–279, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192585`.

Brocas:1991:PCD

[146] J. Brocas and M. Bauwin. Permutational character of dsd mechanisms in heptacoordinate chemistry. *Journal of Mathematical Chemistry*, 6(1): 281–294, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192586`.

Harary:1991:GPP

[147] Frank Harary, Douglas J. Klein, and Tomislav P. Zivković. Graphical properties of polyhexes: Perfect matching vector and forcing. *Journal of Mathematical Chemistry*, 6(1):295–306, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192587`.

Crippen:1991:CDG

[148] Gordon M. Crippen. Chemical distance geometry: Current realization and future projection. *Journal of Mathematical Chemistry*, 6(1): 307–324, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192588`.

Clare:1991:OPC

[149] B. W. Clare and D. L. Kepert. The optimal packing of circles on a sphere. *Journal of Mathematical Chemistry*, 6(1):325–349, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192589`.

Senn:1991:NCS

[150] Peter Senn. Numerical computation of surface areas of molecules. *Journal of Mathematical Chemistry*, 6(1):351–358, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01192590`.

Kern:1991:NBB

[151] A. Kern, H.-J. Krug, and L. Pohlmann. Nucleation in a bistable Belousov–Zhabotinskii system. *Journal of Mathematical Chemistry*, 6(1):

359–375, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01192591.

Gutman:1991:PMR

[152] I. Gutman, J. W. Kennedy, and L. V. Quintas. Perfect matchings in random hexagonal chain graphs. *Journal of Mathematical Chemistry*, 6(1): 377–383, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01192592.

Klein:1991:CAK

[153] D. J. Klein. Comment on average Kekulé-structure counts for random conjugated copolymers. *Journal of Mathematical Chemistry*, 6(1): 385–388, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01192593.

Mezey:1991:EFb

[154] Paul G. Mezey. Editorial foreword. *Journal of Mathematical Chemistry*, 7(1):i, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/BF01200812; http://link.springer.com/article/10.1007/BF01200812.

Johnson:1991:CSE

[155] Mark Johnson, Chun che Tsai, and Victor Nicholson. Chemical stereographs: An extension of chemical graphs for representing stereochemical and conformational structures. *Journal of Mathematical Chemistry*, 7(1):3–38, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01200813.

Mezey:1991:DST

[156] Paul G. Mezey. The degree of similarity of three-dimensional bodies: Application to molecular shape analysis. *Journal of Mathematical Chemistry*, 7(1):39–49, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01200814.

King:1991:TAC

[157] R. B. King. Topological aspects of chemically significant polyhedra. *Journal of Mathematical Chemistry*, 7(1):51–68, December 1991. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200815`.

King:1991:ETC

[158] R. B. King. Experimental tests of chirality algebra. *Journal of Mathematical Chemistry*, 7(1):69–84, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200816`.

Whittington:1991:TDC

[159] S. G. Whittington, C. E. Soteros, and N. Madras. Temperature dependence of the configurational free energy of a branched polymer. *Journal of Mathematical Chemistry*, 7(1):87–94, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200817`.

Tachibana:1991:SMC

[160] Akitomo Tachibana. String model of chemical reaction coordinate. *Journal of Mathematical Chemistry*, 7(1):95–110, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200818`.

Fujita:1991:EOR

[161] Shinsaku Fujita. Enumeration of organic reactions by counting substructures of imaginary transition structures. Importance of orbits governed by coset representations. *Journal of Mathematical Chemistry*, 7(1):111–133, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200819`.

Klin:1991:GTA

[162] Mikhail H. Klin, Serge S. Tratch, and Nikolai S. Zefirov. Group-theoretical approach to the investigation of reaction graphs for highly degenerate rearrangements of chemical compounds I. Criterion of the connectivity of a graph. *Journal of Mathematical Chemistry*, 7(1):135–151, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200820`.

Randic:1991:GMD

[163] Milan Randić. Generalized molecular descriptors. *Journal of Mathematical Chemistry*, 7(1):155–168, December 1991. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200821`.

Rouvray:1991:PMF

[164] D. H. Rouvray and H. Kumazaki. Prediction of molecular flexibility in halogenated alkanes via fractal dimensionality. *Journal of Mathematical Chemistry*, 7(1):169–185, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200822`.

Klopman:1991:GTB

[165] Gilles Klopman and Robert V. Henderson. A graph theory-based "expert system" methodology for structure-activity studies. *Journal of Mathematical Chemistry*, 7(1):187–216, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200823`.

Oyama:1991:ASC

[166] Mayumi Oyama, Shin ichi Sasaki, and Mototsugu Yoshida. Application of the stepwise clustering method for efficient drawing of biopolymer structures. *Journal of Mathematical Chemistry*, 7(1):217–227, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200824`.

Kier:1991:IES

[167] Lemont B. Kier, Lowell H. Hall, and Jack W. Frazer. An index of electrotopological state for atoms in molecules. *Journal of Mathematical Chemistry*, 7(1):229–241, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200825`.

Basak:1991:PPM

[168] Subhash C. Basak, Gerald J. Niemi, and Gilman D. Veith. Predicting properties of molecules using graph invariants. *Journal of Mathematical Chemistry*, 7(1):243–272, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200826`.

Doweyko:1991:HAS

[169] A. M. Doweyko. The hypothetical active site lattice — in vitro and in vivo explorations using a three-dimensional QSAR technique. *Journal of Mathematical Chemistry*, 7(1):273–285, December 1991. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200827`.

Hosoya:1991:FRR

[170] Haruo Hosoya. Factorization and recursion relations of the matching and characteristic polynomials of periodic polymer networks. *Journal of Mathematical Chemistry*, 7(1):289–305, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200828`.

Abe:1991:CAG

[171] Hidetsugu Abe, Sae Takahashi, and Shin ichi Sasaki. Computer-aided generation of IUPAC nomenclatures for acyclic compounds. *Journal of Mathematical Chemistry*, 7(1):307–324, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200829`.

Mizoguchi:1991:HMC

[172] Noriyuki Mizoguchi. Hückel and Möbius cyclic conjugated molecules. *Journal of Mathematical Chemistry*, 7(1):325–340, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200830`.

Sato:1991:HGR

[173] M. Sato. Hamiltonian graph representation of zeolite frameworks and Si, Al ordering in the framework. *Journal of Mathematical Chemistry*, 7(1):341–352, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200831`.

Balasubramanian:1991:GTP

[174] K. Balasubramanian. Graph theory and the PPP method. *Journal of Mathematical Chemistry*, 7(1):353–362, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200832`.

Muller:1991:RTS

[175] Anna Muller. Reassessing the transformation step in factor theory. The case for a non-orthogonal transformation matrix. *Journal of Mathematical Chemistry*, 7(1):363–383, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01200833`.

Anonymous:1991:EF

[176] Anonymous. Editorial foreword. *Journal of Mathematical Chemistry*, 8(1):vii, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01166919; http://link.springer.com/article/10.1007/BF01166919`.

Delest:1991:PAS

[177] M. Delest. Polyominoes and animals: Some recent results. *Journal of Mathematical Chemistry*, 8(1):3–18, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166920`.

Zivkovic:1991:GIG

[178] Tomislav P. Zivković. On graph isomorphism and graph automorphism. *Journal of Mathematical Chemistry*, 8(1):19–37, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166921`.

Balinska:1991:SGR

[179] Krystyna T. Balińska and Louis V. Quintas. The sequential generation of random edge maximal f-graphs as a function of f. *Journal of Mathematical Chemistry*, 8(1):39–51, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166922`.

Graovac:1991:WIG

[180] Ante Graovac and Tomaz Pisanski. On the Wiener index of a graph. *Journal of Mathematical Chemistry*, 8(1):53–62, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166923`.

Cyvin:1991:PTA

[181] S. J. Cyvin, J. Brunvoll, and B. N. Cyvin. A periodic table for all-benzenoid hydrocarbons and enumerations of some polyrex isomers. *Journal of Mathematical Chemistry*, 8(1):63–75, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166924`.

Kirby:1991:RSF

[182] E. C. Kirby. On the recognition of structural features: Some general problems illustrated by Hamiltonian paths in polyhexes. *Journal*

of Mathematical Chemistry, 8(1):77–87, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166925`.

Mezey:1991:HHP

[183] Paul G. Mezey. The α, β, γ-Hull and the T-hull of a point set: Tools for the analysis of shapes and relative orientations of objects in 3d-space. *Journal of Mathematical Chemistry*, 8(1):91–102, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166926`.

Ponec:1991:TAC

[184] Robert Ponec and Martin Strnad. Topological aspects of chemical reactivity. *Journal of Mathematical Chemistry*, 8(1):103–112, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166927`.

Plavsic:1991:CCM

[185] D. Plavsić, S. Nikolić, and N. Trinajstić. The conjugated-circuit model: The optimum parameters for benzenoid hydrocarbons. *Journal of Mathematical Chemistry*, 8(1):113–120, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166928`.

Fabic-Petrac:1991:SCR

[186] I. Fabič-Petrač, B. Jerman-Blazič, and V. Batagelj. Study of computation, relatedness and activity prediction of topological indices. *Journal of Mathematical Chemistry*, 8(1):121–134, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166929`.

Djrasovic:1991:LPA

[187] M. Djrasović, S. Grubacić, and Z. Stipcević. A list-processing approach to quantum mechanics. *Journal of Mathematical Chemistry*, 8(1):137–150, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166930`.

Surjan:1991:NSE

[188] Péter R. Surján. Nonlinear Schrödinger equations and intermolecular interactions. *Journal of Mathematical Chemistry*, 8(1):151–160,

December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166931.

Ptak:1991:DET

[189] W. S. Ptak, J. Giemza, and K. Tkacz. Differential equations for total energy of atoms and atomic ions within Thomas–Fermi approximation. *Journal of Mathematical Chemistry*, 8(1):161–168, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166932.

Cioslowski:1991:POO

[190] J. Cioslowski. Partitioning of the orbital overlap matrix and the localization criteria. *Journal of Mathematical Chemistry*, 8(1):169–178, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166933.

Klasing:1991:PCD

[191] L. Klasing, Lj. Pasa Tolić, H. Spiegl, J. V. Knop, and S. P. McGlynn. Positional and conformational dependence of long-range interactions in 3, 16- and 3, 17-androstanediones. *Journal of Mathematical Chemistry*, 8(1):179–184, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166934.

Vikic-Topic:1991:MDL

[192] D. Vikić-Topić, C. L. Khetrapal, G. R. Christie, P. Sandor, and Z. Meić. On the models for deuterium long-range isotope effects in ^{13}C NMR spectroscopy. *Journal of Mathematical Chemistry*, 8(1):185–192, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166935.

Buyukbingol:1991:NPM

[193] Erdem Buyukbingol and Gilles Klopman. A new proposed model of aldose reductase enzyme inhibition on the basis of an artificial intelligence approach: A computer automated structure evaluation (case) study. *Journal of Mathematical Chemistry*, 8(1):195–205, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166936.

Mintas:1991:MMC

[194] Mladen Mintas, Nenad Raos, and Albrecht Mannschreck. Molecular-mechanics calculations of the geometry and racemization energies of an *N*-aryl-2(1H)-quinolone and *N*-aryl-4-pyridones. *Journal of Mathematical Chemistry*, 8(1):207–216, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166937`.

Luo:1991:ACV

[195] Ning Luo, Masayuki Shibata, and Robert Rein. An algorithm for converting a virtual-bond chain into a complete polypeptide backbone chain. *Journal of Mathematical Chemistry*, 8(1):217–227, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166938`.

Juretic:1991:PSS

[196] Davor Juretić and Robert W. Williams. Protein secondary structure preferencs. *Journal of Mathematical Chemistry*, 8(1):229–242, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166939`.

Borstnik:1991:PRC

[197] B. Borstnik and D. Lukman. Percolation of randomly centered rods and spheres. *Journal of Mathematical Chemistry*, 8(1):245–254, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166940`.

Brak:1991:BCL

[198] R. Brak, A. J. Guttmann, and S. G. Whittington. On the behaviour of collapsing linear and branched polymers. *Journal of Mathematical Chemistry*, 8(1):255–267, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166941`.

Radic-Peric:1991:CPF

[199] Jelena Radić-Perić. Calculation of partition functions of tetra-atomic molecules. *Journal of Mathematical Chemistry*, 8(1):269–279, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166942`.

Jeftic:1991:AOM

[200] Jelena Jeftić and Tomislav Cvitas. Analysis of ozone monitoring data. *Journal of Mathematical Chemistry*, 8(1):283–289, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166943`.

Jelmert:1991:PSR

[201] T. A. Jelmert. Properties of the square-root derivative type curve. *Journal of Mathematical Chemistry*, 8(1):291–305, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166944`.

Gund:1991:MMS

[202] Tamara M. Gund, Kanhiya Shukla, and Tsung-Ping Su. Molecular modeling of sigma receptor ligands: A model of binding based on conformational and electrostatic considerations. *Journal of Mathematical Chemistry*, 8(1):309–325, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166945`.

Trofimov:1991:OPC

[203] Michael I. Trofimov. An optimization of the procedure for the calculation of Hosoya's index. *Journal of Mathematical Chemistry*, 8(1):327–332, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166946`.

Ellzey:1991:ERM

[204] M. L. Ellzey, Jr. Expression of the SU(2) rotation matrices $D^{(j)}$ in terms of normalized irreducible tensorial matrices. *Journal of Mathematical Chemistry*, 8(1):333–344, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166947`.

Rowlinson:1991:CPS

[205] Peter Rowlinson. On the characteristic polynomials of spirographs and related graphs. *Journal of Mathematical Chemistry*, 8(1):345–354, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166948`.

Gutman:1991:EPT

[206] I. Gutman, R. B. Mallion, and D. H. Rouvray. Extension of the pairing theorem to Möbius non-alternant hydrocarbons. *Journal of Mathematical Chemistry*, 8(1):355–366, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166949`.

Demirev:1991:CNC

[207] Plamen A. Demirev, Alexander S. Dyulgerov, and Ivan P. Bangov. CTI: A novel charge-related topological index with low degeneracy. *Journal of Mathematical Chemistry*, 8(1):367–382, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166950`.

Balaban:1991:NVI

[208] Alexandru T. Balaban and Teodor-Silviu Balaban. New vertex invariants and topological indices of chemical graphs based on information on distances. *Journal of Mathematical Chemistry*, 8(1):383–397, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166951`.

Mallion:1991:PGJ

[209] R. B. Mallion and D. H. Rouvray. Postcript to "The golden jubilee of the Coulson–Rushbrooke pairing theorem". *Journal of Mathematical Chemistry*, 8(1):399–400, December 1991. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01166952; http://link.springer.com/article/10.1007/BF01166952`. See [103].

Ugi:1992:AGT

[210] Ivar Ugi and Alf Dengler. The algebraic and graph theoretical completion of truncated reaction equations. *Journal of Mathematical Chemistry*, 9(1):1–10, March 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01172925`.

Xiaofeng:1992:ICP

[211] Guo Xiaofeng and Zhang Fuji. An improvement of the canonical P–V path elimination for recognizing Kekuléan benzenoid systems. *Journal of Mathematical Chemistry*, 9(1):11–17, March 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01172926`.

Cyvin:1992:HRN

[212] S. J. Cyvin, J. Brunvoll, and B. N. Cyvin. Harary–Read numbers for catafusenes: Complete classification according to symmetry. *Journal of Mathematical Chemistry*, 9(1):19–31, March 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01172927`.

Cyvin:1992:GFH

[213] S. J. Cyvin and J. Brunvoll. Generating functions for the Harary–Read numbers classified according to symmetry. *Journal of Mathematical Chemistry*, 9(1):33–38, March 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01172928`.

Nord:1992:EML

[214] R. S. Nord. The end-on mechanism for lattice filling: Comparison with the conventional mechanism and application to the car-parking problem. *Journal of Mathematical Chemistry*, 9(1):39–53, March 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01172929`.

Zivkovic:1992:ERG

[215] Tomislav P. Zivković. Eigenvalues of the real generalized eigenvalue equation perturbed by a low-rank perturbation. *Journal of Mathematical Chemistry*, 9(1):55–73, March 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01172930`.

Bonchev:1992:TAI

[216] Danail Bonchev and Lemont B. Kier. Topological atomic indices and the electronic charges in alkanes. *Journal of Mathematical Chemistry*, 9(1):75–85, March 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01172931`.

Echave:1992:BCH

[217] Julián Echave and Francisco M. Fernández. Baker–Campbell–Hausdorff relations for finite-dimensional Lie algebras. *Journal of Mathematical Chemistry*, 9(1):87–94, March 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01172932`.

Randic:1992:SSI

[218] Milan Randić. In search of structural invariants. *Journal of Mathematical Chemistry*, 9(2):97–146, June 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164840`.

Rayens:1992:BCO

[219] William S. Rayens. Barycentric coordinates and the orientation of the classical mixture surface. *Journal of Mathematical Chemistry*, 9 (2):147–160, June 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164841`.

Bytheway:1992:MMC

[220] Ian Bytheway and David L. Kepert. The mathematical modelling of cluster geometry. *Journal of Mathematical Chemistry*, 9(2):161–180, June 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164842`.

Kvasnicka:1992:IMC

[221] V. Kvasnička and J. Pospíchal. An improved method of constructive enumeration of graphs. *Journal of Mathematical Chemistry*, 9 (2):181–196, June 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164843`.

Csavinszky:1992:BEA

[222] P. Csavinszky and H. Oyoko. Binding energies of on-axis hydrogenic and nonhydrogenic donors in GaAs/$Ga_{1-x}Al_xAs$. *Journal of Mathematical Chemistry*, 9(3):197–206, September 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165147`.

Rucker:1992:UPI

[223] Christoph Rücker and Gerta Rücker. Understanding the properties of isospectral points and pairs in graphs: The concept of orthogonal relation. *Journal of Mathematical Chemistry*, 9(3):207–238, September 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165148`.

Dobrynin:1992:GUH

[224] A. A. Dobrynin. Graphs of unbranched hexagonal systems with equal values of the Wiener index and different numbers of rings. *Journal of Mathematical Chemistry*, 9(3):239–252, September 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165149`.

Dias:1992:ASC

[225] Jerry Ray Dias. Algebraic structure count. *Journal of Mathematical Chemistry*, 9(3):253–260, September 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165150`.

Babic:1992:IBG

[226] D. Babić and I. Gutman. On isospectral benzenoid graphs. *Journal of Mathematical Chemistry*, 9(3):261–278, September 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165151`.

Guo:1992:MPS

[227] Xiaofeng Guo and Fuji Zhang. Mathematical properties and structures of sets of sextet patterns of generalized polyhexes. *Journal of Mathematical Chemistry*, 9(3):279–290, September 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165152`.

Kozlowski:1992:NDM

[228] Pawel M. Kozlowski. Note on the density matrix for an arbitrary number of closed shells in a bare Coulomb field. *Journal of Mathematical Chemistry*, 9(3):291–294, September 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165153`.

Kunz:1992:MIU

[229] Milan Kunz. A Möbius inversion of the Ulam subgraphs conjecture. *Journal of Mathematical Chemistry*, 9(4):297–305, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166094`.

Simon:1992:RLM

[230] Peter L. Simon. The reversible LVA model. *Journal of Mathematical Chemistry*, 9(4):307–322, December 1992. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166095`.

Farkas:1992:UPR

[231] Henrik Farkas and Peter L. Simon. Use of the parametric representation method in revealing the root structure and Hopf bifurcation. *Journal of Mathematical Chemistry*, 9(4):323–339, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166096`.

Turker:1992:UBL

[232] Lemi Türker. An upper bound for the largest eigenvalue of a graph: Effect of types of vertices. *Journal of Mathematical Chemistry*, 9(4):341–349, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166097`.

Mercier:1992:IRS

[233] Christiane Mercier, Yves Sobel, and Jacques-Emile Dubois. Impact of regularity in structure-property relationships. *Journal of Mathematical Chemistry*, 9(4):351–357, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166098`.

Kolossvary:1992:DHM

[234] István Kolossváry and Colin McMartin. On the degeneracy of the Hessian matrix. *Journal of Mathematical Chemistry*, 9(4):359–367, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166099`.

Pota:1992:ENC

[235] G. Póta. Exact necessary conditions for oscillatory behaviour in a class of closed isothermal reaction systems. *Journal of Mathematical Chemistry*, 9(4):369–372, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166100`.

Trinajstic:1992:CP

[236] Nenad Trinajstić. On the classification of polyhexes. *Journal of Mathematical Chemistry*, 9(4):373–380, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166101`.

Nikolic:1992:CPE

[237] Sonja Nikolić, Dejan Plavsić, and Nenad Trinajstić. On the z-counting polynomial for edge-weighted graphs. *Journal of Mathematical Chemistry*, 9(4):381–387, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166102`.

Cyvin:1992:GEH

[238] S. J. Cyvin. Generalization of extremal hexagonal animals (polyhexes). *Journal of Mathematical Chemistry*, 9(4):389–390, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01166103; http://link.springer.com/article/10.1007/BF01166103`.

Surjan:1992:EF

[239] Peter R. Surján, Gábor Náray-Szabó, Paul G. Mezey, and Nenad Trinajstić. Editorial foreword. *Journal of Mathematical Chemistry*, 10(1): vii–viii, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01169167; http://link.springer.com/article/10.1007/BF01169167`.

Adams:1992:PUS

[240] William H. Adams. The problem of unphysical states in the theory of intermolecular interactions. *Journal of Mathematical Chemistry*, 10 (1):1–23, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169168`.

Huzinaga:1992:EHM

[241] S. Huzinaga, S. Katsuki, and O. Matsuoka. Effective Hamiltonian method for environmental effects. *Journal of Mathematical Chemistry*, 10 (1):25–39, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169169`.

Seijo:1992:SCE

[242] Luis Seijo and Zoila Barandiarán. Self-consistent embedded clusters: Building block equations for localized orthogonal orbitals. *Journal of Mathematical Chemistry*, 10(1):41–56, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169170`.

Mehler:1992:SCN

[243] Ernest L. Mehler. Self-consistent, nonorthogonal group function approximation: An ab initio approach for modelling interacting fragments and environmental effects. *Journal of Mathematical Chemistry*, 10(1): 57–91, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169171`.

Angyan:1992:CTF

[244] János G. Ángyán. Common theoretical framework for quantum chemical solvent effect theories. *Journal of Mathematical Chemistry*, 10(1): 93–137, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169172`.

Tapia:1992:SET

[245] O. Tapia. Solvent effect theories: Quantum and classical formalisms and their applications in chemistry and biochemistry. *Journal of Mathematical Chemistry*, 10(1):139–181, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169173`.

Miertus:1992:CME

[246] Stanislav Miertus and Vladimir Frecer. Continuum models of environmental effects on molecular structure and mechanisms in chemistry and biology. *Journal of Mathematical Chemistry*, 10(1):183–204, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169174`.

Roeggen:1992:EDA

[247] Inge Røeggen. An energy decomposition analysis of intermolecular interactions. *Journal of Mathematical Chemistry*, 10(1):205–220, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169175`.

Hansen:1992:CSI

[248] Aage E. Hansen and Thomas D. Bouman. Chromophores in spectroscopy: Ab initio studies of localized descriptions of molecular electronic excitations. *Journal of Mathematical Chemistry*, 10(1):221–247, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169176.

Peluso:1992:TAE

[249] Andrea Peluso, Carlo Adamo, and Giuseppe Del Re. A theoretical analysis of excited state proton transfer in 3-hydroxyflavone. Promoting effect of a low frequency bending mode. *Journal of Mathematical Chemistry*, 10(1):249–274, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169177.

Silvi:1992:MLD

[250] B. Silvi, V. Chandrasekharan, M. E. Alikhani, and R. D. Etters. Modelling light diatomics trapped in rare gas matrices: H_2, HD and D_2 in Ar, Kr and Xe. *Journal of Mathematical Chemistry*, 10(1):275–302, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169178.

Laszlo:1992:EPA

[251] István László. Embedding by pseudo atoms, and the topologically determined one-electronic energy levels. *Journal of Mathematical Chemistry*, 10(1):303–311, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169179.

Kurti:1992:EUC

[252] Jenö Kürti and Péter R. Surján. Embedded units in conjugated polymers. *Journal of Mathematical Chemistry*, 10(1):313–327, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169180.

Arteca:1992:CDM

[253] Gustav A. Arteca and Paul G. Mezey. Configurational dependence of molecular shape. *Journal of Mathematical Chemistry*, 10(1):329–371, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169181.

Mezey:1992:EF

[254] Paul G. Mezey and Nenad Trinajstić. Editorial foreword. *Journal of Mathematical Chemistry*, 11(1):i, December 1992. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01164190; http://link.springer.com/article/10.1007/BF01164190`.

Baraglia:1992:MPA

[255] R. Baraglia, R. Ferrini, D. Laforenza, R. Perego, A. Laganà, and O. Gervasi. A massively parallel approach to the quasiclassical reactive scattering. *Journal of Mathematical Chemistry*, 11(1):1–11, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164191`.

Kibler:1992:QGT

[256] Maurice Kibler and Tidjani Négadi. On quantum groups and their potential use in mathematical chemistry. *Journal of Mathematical Chemistry*, 11(1):13–25, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164192`.

Mezey:1992:SAT

[257] Paul G. Mezey. Similarity analysis in two and three dimensions using lattice animals and polycubes. *Journal of Mathematical Chemistry*, 11 (1):27–45, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164193`.

Nicholson:1992:ARM

[258] Victor A. Nicholson and Gerald M. Maggiora. An augmented ribbon model of protein structure. *Journal of Mathematical Chemistry*, 11(1): 47–63, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164194`.

Babaev:1992:RTG

[259] Eugeny V. Babaev and Nikolai S. Zefirov. Ring-transformation graphs and their application to degenerate heterocyclic rearrangements. *Journal of Mathematical Chemistry*, 11(1):65–78, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164195`.

Balaban:1992:CGA

[260] Teodor Silviu Balaban, Petru A. Filip, and Ovidiu Ivanciuc. Computer generation of acyclic graphs based on local vertex invariants and topological indices. Derived canonical labelling and coding of trees and alkanes.

Journal of Mathematical Chemistry, 11(1):79–105, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164196`.

Bonchev:1992:TAM

[261] D. Bonchev, O. Mekenyan, and V. Kamenska. A topological approach to the modelling of polymer properties (the tempo method). *Journal of Mathematical Chemistry*, 11(1):107–132, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164197`.

Djurasovic:1992:CNL

[262] M. Djurasović and Z. Stipcević. Combinatorial and noncommutative list-processing and associated graphs. *Journal of Mathematical Chemistry*, 11(1):133–144, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164198`.

Gropp:1992:CRG

[263] Harald Gropp. Configurations, regular graphs and chemical compounds. *Journal of Mathematical Chemistry*, 11(1):145–153, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164199`.

Ivanciuc:1992:NGI

[264] Ovidiu Ivanciuc and Alexandru T. Balaban. Nonisomorphic graphs with identical atomic counts of self-returning walks: Isocodal graphs. *Journal of Mathematical Chemistry*, 11(1):155–167, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164200`.

Ivanciuc:1992:RRC

[265] Ovidiu Ivanciuc and Alexandru T. Balaban. Recurrence relationships for the computation of the number of Kekulé structures. *Journal of Mathematical Chemistry*, 11(1):169–177, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164201`.

Juric:1992:MTI

[266] Albin Jurić, Mirko Gagro, Sonja Nikolić, and Nenad Trinajstić. Molecular topological index: An application in the QSAR study of toxicity of alcohols. *Journal of Mathematical Chemistry*, 11(1):179–186, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164202.

Kirby:1992:CET

[267] E. C. Kirby. Coding and enumeration of trees that can be laid upon a hexagon lattice. *Journal of Mathematical Chemistry*, 11(1):187–197, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164203.

Klein:1992:TCC

[268] D. J. Klein and X. Liu. Theorems for carbon cages. *Journal of Mathematical Chemistry*, 11(1):199–205, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164204.

Lloyd:1992:MPG

[269] E. Keith Lloyd. Marks of permutation groups and isomer enumeration. *Journal of Mathematical Chemistry*, 11(1):207–222, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164205.

Mihalic:1992:DMC

[270] Zlatko Mihalić, Darko Veljan, Dragan Amić, Sonja Nikolić, Dejan Plavsić, and Nenad Trinajstić. The distance matrix in chemistry. *Journal of Mathematical Chemistry*, 11(1):223–258, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164206.

Diudea:1992:MTV

[271] M. V. Diudea, D. Horvath, I. E. Kacso, O. M. Minailiuc, and B. Parv. Molecular topology. VIII: Centricities in molecular graphs. The MOLCEN algorithm. *Journal of Mathematical Chemistry*, 11(1):259–270, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164207.

Sekusak:1992:SSC

[272] Sanja Sekusak and Aleksandar Sabljić. Soil sorption and chemical topology. *Journal of Mathematical Chemistry*, 11(1):271–280, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164208.

Cyvin:1992:EPO

[273] S. J. Cyvin, Fuji Zhang, and J. Brunvoll. Enumeration of perifusenes with one internal vertex: A complete mathematical solution. *Journal of Mathematical Chemistry*, 11(1):283–292, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164209`.

Zhang:1992:EKS

[274] Fuji Zhang and Xiaofeng Guo. The existence of Kekulé structures in helicenes and enumeration of concealed non–Kekuléan helicenes with $h \leq 13$. *Journal of Mathematical Chemistry*, 11(1):293–309, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164210`.

Demiralp:1992:BSC

[275] M. Demiralp, N. A. Baykara, and H. Taseli. A basis set comparison in a variational scheme for the Yukawa potential. *Journal of Mathematical Chemistry*, 11(1):311–323, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164211`.

Kryachko:1992:FRD

[276] Eugene S. Kryachko, Eduardo V. Ludeña, and Toshikatsu Koga. Formulation of N- and v-representable density functional theory. III: Excited states. *Journal of Mathematical Chemistry*, 11(1):325–339, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164212`.

Temme:1992:SMP

[277] F. P. Temme and J. P. Colpa. Summary of S_n mapping properties of some lexical p-tuples, or wordlengths, over $(M_1 - M_2)$ fields of Rota–Cayley algebra in generating Hilbert space $\mathrm{SO}(3) \times S_n$ irreps of higher I_i identical spin clusters, $[A]_n(S_n)$, for $n \leq 7$. *Journal of Mathematical Chemistry*, 11(1):341–352, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164213`.

Kvasnicka:1992:ETM

[278] V. Kvasnicka and J. Pospíchal. An existence theorem for molecular graphs determined by a sequence of valence states. *Journal of Mathematical Chemistry*, 11(1):353–364, December 1992. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164214.

Leroy:1992:SDN

[279] J. P. Leroy, R. Wallace, and H. Rabitz. A strategy to derive new internal coordinates by partitioning the internal configuration space according to invariance properties. *Journal of Mathematical Chemistry*, 11(1): 365–404, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164215.

Stacho:1992:MFG

[280] László L. Stachó and Miklós I. Bán. Mathematical foundation of a global strategy for searching reaction paths. *Journal of Mathematical Chemistry*, 11(1):405–421, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164216.

Anonymous:1992:E

[281] Anonymous. Erratum. *Journal of Mathematical Chemistry*, 11(1):423, December 1992. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/BF01164217; http://link.springer.com/article/10.1007/BF01164217.

Mezey:1993:EFa

[282] Paul G. Mezey and Nenad Trinajstić. Editorial foreword. *Journal of Mathematical Chemistry*, 12(1):i, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/BF01164619; http://link.springer.com/article/10.1007/BF01164619.

Fernandez:1993:QAT

[283] Francisco M. Fernández and Eduardo A. Castro. Quasi-algebraic treatment of bound states of simple one-electron systems. *Journal of Mathematical Chemistry*, 12(1):1–8, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164620.

King:1993:CAT

[284] R. Bruce King. Chemical applications of topology and group theory. 26. The sextuple diamond–square–diamond rearrangement of the icosahedron through a cuboctahedron intermediate. *Journal of Mathematical*

Chemistry, 12(1):9–16, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164621`.

Taylor:1993:FCG

[285] Keith F. Taylor and Shigeru Arimotol. The functional calculus and a generalization of the Coulson–Rushbrooke pairing theorem. *Journal of Mathematical Chemistry*, 12(1):17–27, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164622`.

Cioslowski:1993:ETE

[286] Jerzy Cioslowski and Stacey T. Mixon. Exact topological π-electron Hamiltonians from ab initio wavefunctions? *Journal of Mathematical Chemistry*, 12(1):29–36, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164623`.

Arteca:1993:SLS

[287] Gustavo A. Arteca. Small- and large-scale global shape features in macromolecular backbones. *Journal of Mathematical Chemistry*, 12(1):37–51, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164624`.

Nicholson:1993:PGA

[288] Victor Nicholson and John P. Neuzil. The projection graph of the augmented ribbon model is unique. *Journal of Mathematical Chemistry*, 12(1):53–58, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164625`.

Chartrand:1993:RCT

[289] Gary Chartrand, Héctor Hevia, and Mark A. Johnson. A representation of chemical transformations by labeled graphs. *Journal of Mathematical Chemistry*, 12(1):59–80, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164626`.

Klein:1993:RD

[290] D. J. Klein and M. Randić. Resistance distance. *Journal of Mathematical Chemistry*, 12(1):81–95, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164627`.

Chou:1993:GRN

[291] Kuo-Chen Chou. Graphic rule for non-steady-state enzyme kinetics and protein folding kinetics. *Journal of Mathematical Chemistry*, 12(1): 97–108, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164628`.

Brunvoll:1993:MAE

[292] J. Brunvoll, B. N. Cyvin, and S. J. Cyvin. More about extremal animals. *Journal of Mathematical Chemistry*, 12(1):109–119, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164629`.

Lee:1993:EEG

[293] Shyi-Long Lee and Yeong-Nan Yeh. On eigenvalues and eigenvectors of graphs. *Journal of Mathematical Chemistry*, 12(1):121–135, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164630`.

Babic:1993:IBG

[294] D. Babić. Isospectral benzenoid graphs with an odd number of vertices. *Journal of Mathematical Chemistry*, 12(1):137–146, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164631`.

Chen:1993:CCS

[295] Rong si Chen and Xiao feng Guo. k-coverable coronoid systems. *Journal of Mathematical Chemistry*, 12(1):147–162, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164632`.

Guo:1993:EAG

[296] Xiao feng Guo and Fuji Zhang. An efficient algorithm for generating all Kekulé patterns of a generalized benzenoid system. *Journal of Mathematical Chemistry*, 12(1):163–171, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164633`.

Fujita:1993:EDG

[297] Shinsaku Fujita. Enumeration of digraphs with a given automorphism group. *Journal of Mathematical Chemistry*, 12(1):173–195, De-

cember 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164634`.

Gutman:1993:EHC

[298] Ivan Gutman. Extremal hexagonal chains. *Journal of Mathematical Chemistry*, 12(1):197–210, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164635`.

Hosoya:1993:MPT

[299] Haruo Hosoya and Frank Harary. On the matching properties of three fence graphs. *Journal of Mathematical Chemistry*, 12(1):211–218, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164636`.

Zhang:1993:MCP

[300] Hongxing Zhang and K. Balasubramanian. Moments and characteristic polynomials for square lattice graphs. *Journal of Mathematical Chemistry*, 12(1):219–234, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164637`.

Plavsic:1993:HIC

[301] Dejan Plavsić, Sonja Nikolić, Nenad Trinajstić, and Zlatko Mihalić. On the Harary index for the characterization of chemical graphs. *Journal of Mathematical Chemistry*, 12(1):235–250, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164638`.

Nikolic:1993:MTI

[302] Sonja Nikolić, Nenad Trinajstić, and Zlatko Mihalid. Molecular topological index: An extension to heterosystems. *Journal of Mathematical Chemistry*, 12(1):251–264, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164639`.

Mizoguchi:1993:GCR

[303] Noriyuki Mizoguchi. Graphs corresponding to reference polynomial or to circuit characteristic polynomial. *Journal of Mathematical Chemistry*, 12(1):265–277, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164640`.

Gao:1993:TFG

[304] Ying-Duo Gao, Hitomi Kumazaki, Junko Terai, Kanako Chida, and Haruo Hosoya. Topological factors governing the HOMO–LUMO band gap of the density of states of periodic hydrocarbon polymer networks. *Journal of Mathematical Chemistry*, 12(1):279–308, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164641`.

Ivanciuc:1993:DTI

[305] Ovidiu Ivanciuc, Teodor-Silviu Balaban, and Alexandru T. Balaban. Design of topological indices. Part 4. Reciprocal distance matrix, related local vertex invariants and topological indices. *Journal of Mathematical Chemistry*, 12(1):309–318, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164642`.

Sinanoglu:1993:AOG

[306] Oktay Sinanoglu. Autocatalytic and other general networks for chemical mechanisms, pathways, and cycles: Their systematic and topological generation. *Journal of Mathematical Chemistry*, 12(1):319–363, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164643`.

Mezey:1993:TSA

[307] Paul G. Mezey. Topological shape analysis of chain molecules: An application of the GSTE principle. *Journal of Mathematical Chemistry*, 12(1):365–373, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164644`.

Mezey:1993:EFb

[308] Paul G. Mezey and Nenad Trinajstić. Editorial foreword. *Journal of Mathematical Chemistry*, 13(1):vii, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01165547; http://link.springer.com/article/10.1007/BF01165547`.

Rivier:1993:EG

[309] Nicolas Rivier. Entanglements in glass. *Journal of Mathematical Chemistry*, 13(1):1–14, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165548`.

Herman:1993:MDM

[310] Michael F. Herman and Ping Tong. Models for the dynamics of monodisperse polymer melts based on lateral chain motions. *Journal of Mathematical Chemistry*, 13(1):15–32, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165549`.

Chirico:1993:TML

[311] Giuseppe Chirico, Ulrike Kapp, Konstanin Klenin, Werner Kremer, and Jörg Langowski. Ten microseconds in the life of a superhelix. *Journal of Mathematical Chemistry*, 13(1):33–43, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165550`.

Schill:1993:TYI

[312] G. Schill. Thirty years of investigations in the field of catenanes, rotaxanes and knots. *Journal of Mathematical Chemistry*, 13(1):45–46, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01165551; http://link.springer.com/article/10.1007/BF01165551`.

Logemann:1993:RMM

[313] Enno Logemann. Real molecules as models for mathematical chemistry. *Journal of Mathematical Chemistry*, 13(1):47–51, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165552`.

Littke:1993:RMM

[314] Walter Littke and Enno Logemann. Real molecules as models for mathematical chemistry. *Journal of Mathematical Chemistry*, 13(1):53–57, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165553`.

Mezey:1993:DSA

[315] Paul G. Mezey. Dynamic shape analysis of molecules in restricted domains of a configuration space. *Journal of Mathematical Chemistry*, 13(1):59–70, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165554`.

Easthope:1993:CCC

[316] Peter L. Easthope. Classifying the conformations of a chemical system using matrices of integers. *Journal of Mathematical Chemistry*, 13(1): 73–94, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165555`.

Morales:1993:SBC

[317] Daniel A. Morales and Oswaldo Araujo. On the search for the best correlation between graph theoretical invariants and physicochemical properties. *Journal of Mathematical Chemistry*, 13(1):95–106, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165556`.

Kapuy:1993:USS

[318] Ede Kapuy and Cornelia Kozmutza. On the use of spatial symmetry in ab initio calculations. Transformation of the two-electron integrals from atomic orbital to localized molecular orbital basis. *Journal of Mathematical Chemistry*, 13(1):107–113, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165557`.

Dubickas:1993:ALF

[319] Arturas K. Dubickas and A. A. Petraaskas. Application of the linear free energy principle for derivation of nonlinear quantitative structure-activity relationships. A steady-state kinetic model. *Journal of Mathematical Chemistry*, 13(1):115–132, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165558`.

Desainte-Catherine:1993:HGP

[320] M. Desainte-Catherine. A honeycomb graph perfect matchings enumeration. *Journal of Mathematical Chemistry*, 13(1):133–143, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165559`.

Kunz:1993:TGD

[321] Milan Kunz. On topological and geometrical distance matrices. *Journal of Mathematical Chemistry*, 13(1):145–151, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165560`.

Temme:1993:GFS

[322] F. P. Temme. On general forms for structure of some $[n-1,1] \otimes [\lambda] L_{nn}$ inner tensor products with $6 \leq n \leq 20$, (60) for n even, in the context of spin cluster problems of multiquantum NMR. *Journal of Mathematical Chemistry*, 13(1):153–165, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165561`.

Freedman:1993:FRO

[323] Richard W. Freedman and Fred Gornick. Further reflections on the one-dimensional packing problem. *Journal of Mathematical Chemistry*, 13(1): 167–176, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165562`.

Tone:1993:CAT

[324] A. Tone, L. Lain, and J. Millan. Contraction algorithms for third-order reduced density matrices: Symmetric group approach. *Journal of Mathematical Chemistry*, 13(1):177–189, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165563`.

Hall:1993:EDA

[325] George G. Hall. Eigenvalue distributions in alternant hydrocarbons. *Journal of Mathematical Chemistry*, 13(1):191–203, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165564`.

Zimpel:1993:MPR

[326] Zbigniew Zimpel. The metric properties of the reduced nuclear configuration space: Remarks. *Journal of Mathematical Chemistry*, 13(1): 205–208, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165565`.

Mislow:1993:SSA

[327] Kurt Mislow and Pietro Poggi-Corradini. Shape space of achiral simplexes. *Journal of Mathematical Chemistry*, 13(1):209–211, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165566`.

Gutman:1993:BGE

[328] I. Gutman and S. Marković. Benzenoid graphs with equal maximum eigenvalues. *Journal of Mathematical Chemistry*, 13(1):213–215, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165567`.

Arimoto:1993:ALT

[329] Shigeru Arimoto and Mark Spivakovsky. The asymptotic linearity theorem for the study of additivity problems of the zero-point vibrational energy of hydrocarbons and the total pi-electron energy of alternant hydrocarbons. *Journal of Mathematical Chemistry*, 13(1):217–247, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165568`.

Arimoto:1993:AFG

[330] Shigeru Arimoto and Keith Taylor. Aspects of form and general topology: Alpha space asymptotic linearity theorem and the spectral symmetry of alternants. *Journal of Mathematical Chemistry*, 13(1):249–264, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165569`.

Arimoto:1993:PVA

[331] Shigeru Arimoto and Keith Taylor. Practical version of the asymptotic linearity theorem with applications to the additivity problems of thermodynamic quantities. *Journal of Mathematical Chemistry*, 13(1):265–272, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165570`.

Li:1993:UGTa

[332] Xiangzhu Li and Josef Paldus. Unitary group tensor operator algebras for many-electron systems: II. One- and two-body matrix elements. *Journal of Mathematical Chemistry*, 13(1):273–316, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165571`.

MagelaeSilva:1993:FAC

[333] G. Magela e Silva, L. A. C. Malbouisson, A. Naves de Brito, and J. D. M. Vianna. Functional analysis concepts and Hartree–Fock in-

stability conditions. *Journal of Mathematical Chemistry*, 13(1):317–330, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165572`.

Carbo:1993:NSS

[334] Ramon Carbó and Emili Besalú. Nested summation symbols and perturbation theory. *Journal of Mathematical Chemistry*, 13(1):331–342, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165573`.

Csorvassy:1993:MTS

[335] István Csorvássy, Lajos Tözsér, Levente Kárpáti, and Gábor Náray-Szabó. The molecular transform as a similarity measure. *Journal of Mathematical Chemistry*, 13(1):343–357, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165574`.

Kirby:1993:BGP

[336] Edward C. Kirby and Ivan Gutman. The branching graphs of polyhexes: Some elementary theorems, conjectures and open questions. *Journal of Mathematical Chemistry*, 13(1):359–374, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165575`.

Mezey:1993:EFc

[337] Paul G. Mezey and Nenad Trinajstić. Editorial foreword. *Journal of Mathematical Chemistry*, 14(1):vii, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01164449; http://link.springer.com/article/10.1007/BF01164449`.

Csavinszky:1993:AAN

[338] P. Csavinszky. Attainable accuracy in the numerical integration of the Thomas–Fermi kinetic-energy functional using a modeled electron density. *Journal of Mathematical Chemistry*, 14(1):1–6, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164450`.

Flesia:1993:LMC

[339] S. Flesia. Lattice models for the collapse of branched polymers. *Journal of Mathematical Chemistry*, 14(1):7–20, December 1993. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164451.

Ivanciuc:1993:CGD

[340] Ovidiu Ivanciuc, Teodor-Silviu Balaban, and Alexandru T. Balaban. Chemical graphs with degenerate topological indices based on information on distances. *Journal of Mathematical Chemistry*, 14(1):21–33, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164452.

Juretic:1993:PSS

[341] Davor Juretić, Nenad Trinajstic, and Bono Lucić. Protein secondary structure conformations and associated hydrophobicity scales. *Journal of Mathematical Chemistry*, 14(1):35–45, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164453.

Kinoshita:1993:TFI

[342] Shin'ichi Kinoshita. On the three-fold irregular branched coverings of spatial four-valent graphs and its applications. *Journal of Mathematical Chemistry*, 14(1):47–55, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164454.

Linder:1993:FSM

[343] Bruno Linder and Robert A. Kromhout. A formulation of statistical mechanics of ordered systems. *Journal of Mathematical Chemistry*, 14 (1):57–70, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164455.

McLaughlin:1993:AGF

[344] Kevin W. McLaughlin and Craig M. Bertolucci. Applications of generating functions to polymerization kinetics. 3. General procedure illustrated for propagation with monomer conversion. *Journal of Mathematical Chemistry*, 14(1):71–78, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164456.

Mezey:1993:NRP

[345] Paul G. Mezey. New rules on potential surface topology and critical point search. *Journal of Mathematical Chemistry*, 14(1):79–90, December 1993.

CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164457.

Soteros:1993:LMB

[346] C. E. Soteros. Lattice models of branched polymers with specified topologies. *Journal of Mathematical Chemistry*, 14(1):91–102, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164458.

Whittington:1993:SMT

[347] S. G. Whittington. Statistical mechanics of three-dimensional vesicles. *Journal of Mathematical Chemistry*, 14(1):103–110, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164459.

Balasubramanian:1993:GBE

[348] K. Balasubramanian. Generalization of de Bruijn's extension of Pólya's theorem to all characters. *Journal of Mathematical Chemistry*, 14(1): 113–120, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164460.

Ye:1993:ENF

[349] Yuan-Jie Ye. The extended negative factor counting method for tridiagonal block matrices with cross links. *Journal of Mathematical Chemistry*, 14(1):121–139, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164461.

Ye:1993:AEN

[350] Yuan-Jie Ye and János Ladik. The application of the extended negative factor counting method to deal with the electronic energy levels of pig insulin. *Journal of Mathematical Chemistry*, 14(1):141–152, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164462.

Brocas:1993:DMH

[351] J. Brocas. The dsd model in heptacoordinate stereochemistry: a comparison with experiment. *Journal of Mathematical Chemistry*, 14(1): 153–174, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164463.

Dobrynin:1993:DSM

[352] A. A. Dobrynin. Degeneracy of some matrix graph invariants. *Journal of Mathematical Chemistry*, 14(1):175–184, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164464`.

Sinanoglu:1993:DAMa

[353] Oktay Sinanoglu. Dyad algebra and multiplication of graphs. I. Directed graphs. *Journal of Mathematical Chemistry*, 14(1):185–194, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164465`.

Sinanoglu:1993:DAMb

[354] Oktay Sinanoglu. Dyad algebra and multiplication of graphs. II. Undirected graphs. *Journal of Mathematical Chemistry*, 14(1):195–205, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164466`.

Koga:1993:EFA

[355] Toshikatsu Koga. Energy functional of the axial marginal densit in linear molecules. *Journal of Mathematical Chemistry*, 14(1):207–217, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164467`.

delaVega:1993:AEO

[356] J. M. García de la Vega and B. Miguel. Analytic expressions for one-centre p-space integrals over Slater functions. *Journal of Mathematical Chemistry*, 14(1):219–229, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164468`.

Lee:1993:TAS

[357] Shyi-Long Lee and Yeong-Nan Yeh. Topological analysis of some special classes of graphs. II. Steps, ladders, cylinders. *Journal of Mathematical Chemistry*, 14(1):231–241, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164469`.

Randic:1993:GWP

[358] Milan Randić, Keneth J. Kopecky, and Bernadette Baker. Generalized Wheland polynomial for large graphs. *Journal of Mathematical Chemistry*, 14(1):243–258, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164470`.

Quapp:1993:WYT

[359] Wolfgang Quapp and Brenda P. Winnewisser. What you thought you already knew about the bending motion of triatomic molecules. *Journal of Mathematical Chemistry*, 14(1):259–285, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164471`.

Bonchev:1993:CVV

[360] Danail Bonchev and Alexandru T. Balaban. Central vertices versus central rings in polycyclic systems. *Journal of Mathematical Chemistry*, 14(1):287–304, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164472`.

El-Basil:1993:KSG

[361] Sherif El-Basil. Kekulé structures as graph generators. *Journal of Mathematical Chemistry*, 14(1):305–318, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164473`.

Blinder:1993:GUT

[362] S. M. Blinder. Generalized Unsöld theorem and radial distribution function for hydrogenic orbitals. *Journal of Mathematical Chemistry*, 14(1):319–324, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164474`.

Li:1993:UGTb

[363] Xiangzhu Li and Josef Paldus. Unitary group tensor operator algebras for many-electron systems. III. Matrix elements in $\mathrm{U}(n_1+n_2) \supset \mathrm{U}(n_1) \times \mathrm{U}(n_2)$ partitioned basis. *Journal of Mathematical Chemistry*, 14(1):325–355, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164475`.

Kalinichenko:1993:MLI

[364] M. I. Kalinichenko and V. A. Trofitnov. Macrokinetics of laser-induced chemical reactions in gases. *Journal of Mathematical Chemistry*, 14(1): 357–383, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164476`.

Rutherford:1993:GFC

[365] John S. Rutherford. Generating functions for the cage isomers of the C_{20n} icosahedral fullerenes. *Journal of Mathematical Chemistry*, 14(1): 385–390, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164477`.

Bowden:1993:ABD

[366] G. J. Bowden and M. J. Prandolini. Analytical block-diagonalization of matrices using unit spherical tensors. *Journal of Mathematical Chemistry*, 14(1):391–403, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164478`.

Beumee:1993:AMR

[367] Johan G. B. Beumee and Herschel Rabitz. An application of minimax robust optimal control theory for selective vibrational excitation in molecules. *Journal of Mathematical Chemistry*, 14(1):405–425, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164479`.

Weinberg:1993:DFG

[368] Noham Weinberg and Kurt Mislow. Distance functions as generators of chirality measures. *Journal of Mathematical Chemistry*, 14(1):427–450, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164480`.

Zimpel:1993:GAD

[369] Zbigniew Zimpel. A geometrical approach to the degree of chirality and asymmetry. *Journal of Mathematical Chemistry*, 14(1):451–465, December 1993. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164481`.

Liang:1994:AK

[370] Chengzi Liang and Kurt Mislow. On amphicheiral knots. *Journal of Mathematical Chemistry*, 15(1):1–34, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277546`.

Liang:1994:LRC

[371] Chengzhi Liang and Kurt Mislow. A left-right classification of topologically chiral knots. *Journal of Mathematical Chemistry*, 15(1):35–62, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277547`.

Moreira:1994:SCS

[372] Helmar Nunes Moreira and Wang Yuquan. Sufficient conditions for the Sal'nikov equation to have at least two limit cycles. *Journal of Mathematical Chemistry*, 15(1):63–72, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277548`.

Lloyd:1994:CCC

[373] E. Keith Lloyd. Counterexamples to Cyvin's conjecture. *Journal of Mathematical Chemistry*, 15(1):73–76, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277549`.

Butzlaff:1994:HAF

[374] M. Butzlaff, W. Dahmen, S. Diekmann, A. Dress, E. Schmitt, and E. von Kitzing. A hierarchical approach to force field calculations through spline approximations. *Journal of Mathematical Chemistry*, 15 (1):77–92, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277550`.

Hansen:1994:CNB

[375] Pierre Hansen and Maolin Zheng. The Clar number of a benzenoid hydrocarbon and linear programming. *Journal of Mathematical Chemistry*, 15 (1):93–107, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277551`.

Mitin:1994:LEI

[376] Alexander V. Mitin and Gerhard Hirsch. Linear extrapolation in iterative methods. *Journal of Mathematical Chemistry*, 15(1):109–113, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277552`.

Izydorek:1994:NEH

[377] Marek Izydorek, Stawomir Rybicki, and Marietta Kern. A note on the existence of heteroclinic connecting orbits in the Belousov–Zhabotinskii system. *Journal of Mathematical Chemistry*, 15(1):115–121, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277553`.

Morita:1994:SAL

[378] Akio Morita. A simple approach leading to Kramers' turnover on the rate coefficient based on Brownian motion with weak colored dichotomous random force. *Journal of Mathematical Chemistry*, 15(1):123–130, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277554`.

Fernandez:1994:AME

[379] F. M. Fernández and J. F. Ogilvie. Analytic matrix elements of the dipole moment and Herman–Wallis coefficients. *Journal of Mathematical Chemistry*, 15(1):131–142, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277555`.

Terrones:1994:CGM

[380] Humberto Terrones. Curved graphite and its mathematical transformations. *Journal of Mathematical Chemistry*, 15(1):143–156, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277556`.

Terrones:1994:CCP

[381] H. Terrones and A. L. Mackay. The characterisation of coordination polyhedra by invariants. *Journal of Mathematical Chemistry*, 15(1):157–181, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277557`.

Terrones:1994:NCG

[382] H. Terrones and A. L. Mackay. Negatively curved graphite and triply periodic minimal surfaces. *Journal of Mathematical Chemistry*, 15(1): 183–195, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277558`.

Gilat:1994:QCO

[383] G. Gilat. On quantifying chirality — obstacles and problems towards unification. *Journal of Mathematical Chemistry*, 15(1):197–205, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277559`.

Anonymous:1994:ICQ

[384] Anonymous. 8th international Congress of quantum chemistry. *Journal of Mathematical Chemistry*, 15(1):206, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01277560`; `http://link.springer.com/article/10.1007/BF01277560`.

Wawak:1994:GDC

[385] Ryszard J. Wawak, Kenneth D. Gibson, and Harold A. Scheraga. Gradient discontinuities in calculations involving molecular surface area. *Journal of Mathematical Chemistry*, 15(1):207–232, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277561`.

Avery:1994:FTR

[386] John Avery. Fock transforms in reciprocal-space quantum theory. *Journal of Mathematical Chemistry*, 15(1):233–244, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277562`.

Liang:1994:CTC

[387] Chengzhi Liang and Kurt Mislow. Classification of topologically chiral molecules. *Journal of Mathematical Chemistry*, 15(1):245–260, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277563`.

John:1994:AAN

[388] P. E. John and R. B. Malllon. An algorithmic approach to the number of spanning trees in Buckminsterfullerene. *Journal of Mathematical Chemistry*, 15(1):261–271, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277564`.

Yu:1994:AFEa

[389] Hengtai Yu, André Bandrauk, and Vijay Sonnad. Application of the finite element method to time-dependent quantum mechanics: I. H and He in a laser field. *Journal of Mathematical Chemistry*, 15(1):273–286, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277565`.

Yu:1994:AFEb

[390] Hengtai Yu, André D. Bandrauk, and Vijay Sonnad. Application of the finite element method to time-dependent quantum mechanics: II. H_2^+ in a laser field. *Journal of Mathematical Chemistry*, 15(1):287–301, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277566`.

Cassam-Chenai:1994:VSE

[391] P. Cassam-Chenaï. Variational spaces of electronic calculations in quantum chemistry. *Journal of Mathematical Chemistry*, 15(1):303–321, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277567`.

Takeda:1994:ESR

[392] Kyozaburo Takeda. Electronic structure of random copolymers. *Journal of Mathematical Chemistry*, 15(1):323–337, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277568`.

Connolly:1994:AJV

[393] Michael L. Connolly. Adjoint join volumes. *Journal of Mathematical Chemistry*, 15(1):339–352, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277569`.

Glunt:1994:AWC

[394] W. Glunt, T. L. Hayden, C. Wells, J. G. Shelling, and D. J. Ward. Applications of weighting and chirality strategies for distance geometry algorithms to an enterotoxin peptide analog. *Journal of Mathematical Chemistry*, 15(1):353–366, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277570`.

Ashby:1994:IHI

[395] S. J. Ashby, G. J. Bowden, and M. J. Prandolini. Irreducible half-integer rank unit spherical tensors. *Journal of Mathematical Chemistry*, 15(1): 367–387, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277571`.

Brocas:1994:RGC

[396] J. Brocas. The reaction graph of the Cope rearrangement in bullvalene. *Journal of Mathematical Chemistry*, 15(1):389–395, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277572`.

Besalu:1994:GRS

[397] Emili Besalú and Ramon Carbó. Generalized Rayleigh–Schrödinger perturbation theory in matrix form. *Journal of Mathematical Chemistry*, 15(1):397–406, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01277573`.

Mihalic:1994:BGE

[398] Zlatko Mihalić, Darko Babić, and Nenad Trinajstić. Benzenoid graphs with equal maximum eigenvalues. *Journal of Mathematical Chemistry*, 15(1):407, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01277574; http://link.springer.com/article/10.1007/BF01277574`.

Cyvin:1994:GEA

[399] S. J. Cyvin. Generalization of extremal animals once again. *Journal of Mathematical Chemistry*, 15(1):409–410, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01277575; http://link.springer.com/article/10.1007/BF01277575`.

Bowden:1994:CST

[400] G. J. Bowden and M. J. Prandolini. Complete solution for two coupled spin-1/2 nuclei evolving under chemical shift and dipolar interaction. *Journal of Mathematical Chemistry*, 16(1):1–7, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169190`.

Pfalzner:1994:BSP

[401] S. Pfalzner, H. Lehmann, and N. H. March. Bound-state plus continuum electron-densities, and Slater sum, in a bare Coulomb field. *Journal of Mathematical Chemistry*, 16(1):9–18, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169191`.

Maranon:1994:PIF

[402] Julio Marañón. Path integral's formulation of the molecular solvent effects. *Journal of Mathematical Chemistry*, 16(1):19–26, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169192`.

Liang:1994:BL

[403] Chengzhi Liang and Kurt Mislow. On Borromean links. *Journal of Mathematical Chemistry*, 16(1):27–35, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169193`.

Gilat:1994:GPC

[404] G. Gilat and Y. Gordon. Geometric properties of chiral bodies. *Journal of Mathematical Chemistry*, 16(1):37–48, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169194`.

Morita:1994:DPI

[405] Akio Morita. Diffusion processes with inertial effects and with boundary conditions — a solution to the Wang and Uhlenbeck problem. *Journal of Mathematical Chemistry*, 16(1):49–60, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169195`.

Mezei:1994:LRC

[406] Mihaly Mezei and Katalin Bencsáth. Long-range contribution to inverse-distance power and Morse energy and pressure terms of a molecular

liquid, tested on benzene. *Journal of Mathematical Chemistry*, 16(1): 61–71, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169196`.

Gutman:1994:RMF

[407] Ivan Gutman. Rectifying a misbelief: Frank Harary's role in the discovery of the coefficient-theorem in chemical graph theory. *Journal of Mathematical Chemistry*, 16(1):73–78, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169197`.

Campbell:1994:PND

[408] Edwin S. Campbell. Positive and negative domains of vertex-angle space for three-body contributions of several lower order dispersion multipoles. *Journal of Mathematical Chemistry*, 16(1):79–92, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169198`.

Arimoto:1994:STO

[409] Shigeru Arimoto and Paul G. Mezey. Symmorphy transformations and operators in the repeat space $X_r(q)$ for additivity problems. *Journal of Mathematical Chemistry*, 16(1):93–114, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169199`.

Leach:1994:OWB

[410] J. A. Leach, J. H. Merkin, and S. K. Scott. Oscillations and waves in the Belousov–Zhabotinskii reaction in a finite medium. *Journal of Mathematical Chemistry*, 16(1):115–124, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169200`.

Chen:1994:ITA

[411] Jye-Chan Chen, Yu-Chuan Yang, Hsi-Wei Jia, and Tieh-Sheng Lee. Information theoretical analysis of the hydrogen atom. *Journal of Mathematical Chemistry*, 16(1):125–136, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169201`.

Planelles:1994:RHS

[412] Josep Planelles and Pascual Viciano. Reduced Hamiltonians. I: Spin-adapted and spin-nonadapted reduced Hamiltonians. *Journal of Mathe-*

matical Chemistry, 16(1):137–148, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169202`.

Viciano:1994:RHI

[413] Pascual Viciano and Josep Planelles. Reduced Hamiltonians. II: The size-consistency of reduced Hamiltonians defined in model spaces. *Journal of Mathematical Chemistry*, 16(1):149–157, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169203`.

Bracken:1994:SEI

[414] P. Bracken. Small β expansion for infinite chain limit of one dimensional Hubbard model. *Journal of Mathematical Chemistry*, 16(1):159–165, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169204`.

Baykara:1994:ACV

[415] N. A. Baykara and Metin Demiralp. An auto-coherent variational scheme for Yukawa potential. *Journal of Mathematical Chemistry*, 16(1):167–183, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169205`.

Demiralp:1994:OCC

[416] Metin Demiralp and Herschel Rabitz. Optimal control of classical molecular dynamics: A perturbation formulation and the existence of multiple solutions. *Journal of Mathematical Chemistry*, 16(1):185–209, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169206`.

Simek:1994:GPT

[417] Mehmet Simek and Zeynel Yalçin. Generalized Pöschl–Teller potential. *Journal of Mathematical Chemistry*, 16(1):211–215, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169207`.

Roszak:1994:UMP

[418] S. Roszak and K. Balasubramanian. Unresolved mathematical problems in the representation of potential energy surfaces by many-body

potentials. *Journal of Mathematical Chemistry*, 16(1):217–220, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169208`.

Narumi:1994:EPM

[419] Hideyuki Narumi, Hideaki Kita, and Haruo Hosoya. An expression for the perfect matching number of cubic $2 \times m \times n$ lattices and their asymptotic values. *Journal of Mathematical Chemistry*, 16(1): 221–228, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169209`.

Gutman:1994:ICT

[420] I. Gutman, I. Fishtik, and N. Nagypál. An identity in chemical thermodynamics. *Journal of Mathematical Chemistry*, 16(1):229–244, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169210`.

Chauvin:1994:CAF

[421] Remi Chauvin. Chemical algebra. I: Fuzzy subgroups. *Journal of Mathematical Chemistry*, 16(1):245–256, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169211`.

Chauvin:1994:CAIa

[422] Remi Chauvin. Chemical algebra. II: Discriminating pairing products. *Journal of Mathematical Chemistry*, 16(1):257–268, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169212`.

Chauvin:1994:CAIb

[423] Remi Chauvin. Chemical algebra III: Thermochemical approach to completely g-invariant distances. *Journal of Mathematical Chemistry*, 16(1): 269–283, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01169213`.

Chauvin:1994:CAIc

[424] Remi Chauvin. Chemical algebra. IV: "Length" of transformation pathways between skeletal analogs. *Journal of Mathematical Chemistry*, 16(1):285–308, December 1994. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169214.

Elabsy:1994:ENG

[425] A. M. Elabsy and P. Csavinszky. Effect of nonparabolicity of the GaAs conduction band on the binding energy of a hydrogenic donor in a GaAs/$Ga_{1-x}Al_xAs$ quantum dot. *Journal of Mathematical Chemistry*, 16(1): 309–313, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169215.

Leicester:1994:QRMa

[426] Steve Leicester, John Finney, and Robert Bywater. A quantitative representation of molecular surface shape. I: Theory and development of the method. *Journal of Mathematical Chemistry*, 16(1):315–341, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169216.

Leicester:1994:QRMb

[427] Steve Leicester, John Finney, and Robert Bywater. A quantitative representation of molecular surface shape. II: Protein classification using Fourier shape descriptors and classical scaling. *Journal of Mathematical Chemistry*, 16(1):343–365, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169217.

Belger:1994:PVC

[428] M. Belger. Principal vectors of crystallographic groups and applications. *Journal of Mathematical Chemistry*, 16(1):367–388, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01169218.

Anonymous:1994:AAN

[429] Anonymous. An algorithmic approach to the number of spanning trees in Buckminsterfullerene. *Journal of Mathematical Chemistry*, 16(1): 389–390, December 1994. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/BF01169219; http://link.springer.com/article/10.1007/BF01169219.

Wilhelm:1995:SCR

[430] Thomas Wilhelm and Reinhart Heinrich. Smallest chemical reaction system with Hopf bifurcation. *Journal of Mathematical Chemistry*, 17

(1):1–14, February 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165134`.

Hansen:1995:HCH

[431] Pierre Hansen and Maolin Zheng. Hamiltonian circuits, Hamiltonian paths and branching graphs of benzenoid systems. *Journal of Mathematical Chemistry*, 17(1):15–33, February 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165135`.

Weinberg:1995:UCM

[432] Noham Weinberg and Kurt Mislow. A unification of chirality measures. *Journal of Mathematical Chemistry*, 17(1):35–53, February 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165136`.

Vieira:1995:CSH

[433] F. M. C. Vieira and P. M. Bisch. Complete set of Hopf bifurcation in an autocatalytic ring network. *Journal of Mathematical Chemistry*, 17 (1):55–67, February 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165137`.

Duda:1995:TME

[434] Jan Duda and Janina Milewska-Duda. A theoretical model for evaluation of configurational entropy of mixing with respect to shape and size of particles. *Journal of Mathematical Chemistry*, 17(1):69–109, February 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165138`.

Dobrowolski:1995:BET

[435] Jan Cz. Dobrowolski and Michal H. Jamróz. Background elimination in three-dimensional spectroscopy using the intensian method. *Journal of Mathematical Chemistry*, 17(1):111–121, February 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165139`.

Needham:1995:ECC

[436] D. J. Needham and J. H. Merkin. The effects of coupling on chemical wave propagation in quadratic and cubic autocatalysis with decay. *Journal of Mathematical Chemistry*, 17(2):123–137, June 1995. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164844.

Muller:1995:EBN

[437] Andreas Müller and Heinz Kleindienst. Error bounds for the nonrelativistic electronic ground state energy of molecular hydrogen. *Journal of Mathematical Chemistry*, 17(2):139–166, June 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164845.

Aszodi:1995:EPC

[438] András Aszódi and William R. Taylor. Estimating polypeptide α-carbon distances from multiple sequence alignments. *Journal of Mathematical Chemistry*, 17(2):167–184, June 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164846.

Mezey:1995:RCAa

[439] Paul G. Mezey. Rules on chiral and achiral molecular transformations. *Journal of Mathematical Chemistry*, 17(2):185–202, June 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164847.

Walker:1995:NCM

[440] P. Duane Walker and Paul G. Mezey. A new computational microscope for molecules: High resolution MEDLA images of taxol and HIV-1 protease, using additive electron density fragmentation principles and fuzzy set methods. *Journal of Mathematical Chemistry*, 17 (2):203–234, June 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164848.

Chauvin:1995:CAVa

[441] Remi Chauvin. Chemical algebra. V: G-weighted distance extensions and metrics. *Journal of Mathematical Chemistry*, 17(2):235–246, June 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01164849.

Chauvin:1995:CAVb

[442] Remi Chauvin. Chemical algebra. VI: G-weighted metrics of noncompact groups: Group of translations in the Euclidean space. *Journal*

of Mathematical Chemistry, 17(2):247–264, June 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164850`.

Chauvin:1995:CAVc

[443] Remi Chauvin. Chemical algebra. VII: Improper G-weighted metrics of non-compact groups: Lorentz group in the Minkowski space. *Journal of Mathematical Chemistry*, 17(2):265–283, June 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164851`.

Pota:1995:UFM

[444] G. Póta and G. Stedman. An uncommon form of multistationarity in a realistic kinetic model. *Journal of Mathematical Chemistry*, 17 (2):285–289, June 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164852`.

Cyvin:1995:ASN

[445] S. J. Cyvin. Algebraic solution for the numbers of staggered conformers of alkanes. *Journal of Mathematical Chemistry*, 17(2):291–293, June 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164853`.

Li:1995:NAN

[446] Jiabo Li. New algorithm for nonorthogonal ab initio valence bond calculations II: Subgraph-driven method. *Journal of Mathematical Chemistry*, 17(3):295–321, October 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165751`.

Korobov:1995:HCK

[447] A. Korobov. Heterogeneous chemical kinetics: A two-dimensional insight into sigmoid $\alpha - t$ curve. *Journal of Mathematical Chemistry*, 17(3): 323–333, October 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165752`.

Singh:1995:MTT

[448] Tejwant Singh, Rajinder Pal Singh, and Jatinder Dutt. Mass transport to tubular electrodes. *Journal of Mathematical Chemistry*, 17(3): 335–346, October 1995. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165753.

MagelaeSilva:1995:FAC

[449] G. Magela e Silva, L. A. C. Malbouisson, and J. D. M. Vianna. Functional analysis concepts and Hartree–Fock instability conditions II: An analysis of the eight classes of solutions. *Journal of Mathematical Chemistry*, 17 (3):347–355, October 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165754.

Merkin:1995:RDT

[450] J. H. Merkin and M. A. Sadiq. Reaction-diffusion travelling waves in the acidic nitrate–ferroin reaction. *Journal of Mathematical Chemistry*, 17 (3):357–375, October 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165755.

Stacho:1995:TII

[451] László L. Stachó and Miklós I. Bán. Theoretical implications involved in the DDRP method. *Journal of Mathematical Chemistry*, 17(3): 377–393, October 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165756.

Palting:1995:GEM

[452] Pancracio Palting, Shan Tao Lai, and Manzheng Fu. A general expression for matrix elements of reciprocal powers of the displacement coordinate q in the harmonic oscillator basis. *Journal of Mathematical Chemistry*, 17 (3):395–399, October 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165757.

Fernandez:1995:TAP

[453] Ariel Fernández. Towards an action principle governing biopolymer folding in vitro. *Journal of Mathematical Chemistry*, 17(3):401–410, October 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165758.

Liang:1995:TCA

[454] Chengzhi Liang and Kurt Mislow. Topological chirality and achirality of links. *Journal of Mathematical Chemistry*, 18(1):1–24, March 1995.

CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166600.

Guarnieri:1995:TAM

[455] Frank Guarnieri. Theory and algorithms for mixed Monte Carlo-stochastic dynamics simulations. *Journal of Mathematical Chemistry*, 18(1):25–35, March 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166601.

Carbo:1995:DQC

[456] Ramon Carbó and Emili Besalú. Definition and quantum chemical applications of nested summation symbols and logical functions: Pedagogical artificial intelligence devices for formulae writing, sequential programming and automatic parallel implementation. *Journal of Mathematical Chemistry*, 18(1):37–72, March 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166602.

Gutman:1995:GTI

[457] I. Gutman, I. Nagypál, and I. Fishtik. General therodynamic identities for sensitivity coefficients. *Journal of Mathematical Chemistry*, 18 (1):73–82, March 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166603.

Jendrol:1995:LCG

[458] Stanislav Jendrol' and Peter J. Owens. Longest cycles in generalized Buckminsterfullerene graphs. *Journal of Mathematical Chemistry*, 18 (1):83–90, March 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166604.

Temme:1995:MVE

[459] F. P. Temme. On mixed vs. exclusively-bosonic $\left\{ \left[\tilde{\lambda} \right] : p \leq 2^2 \right\}$ (SU2$\times S_n$) irrep sets over $\left\{ \tilde{\mathbf{H}}_v \right\}$ carrier subspaces, in the structure of (SU2 $\times$ S_n $\otimes$ (SU2 $\times$ S_n)$^+$)-derived Liouville space of NMR spin dynamics. *Journal of Mathematical Chemistry*, 18(1):91–95, March 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166605.

Anonymous:1995:E

[460] Anonymous. Erratum. *Journal of Mathematical Chemistry*, 18(1):97–98, March 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/BF01166606; http://link.springer.com/article/10.1007/BF01166606`.

White:1995:SAC

[461] David P. White, P. G. L. Leach, and Neil J. Coville. Solid angles 5. Chiral molecules and the case of face selectivity. *Journal of Mathematical Chemistry*, 18(2):99–114, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164651`.

Cash:1995:FCA

[462] Gordon G. Cash. A fast computer algorithm for finding the permanent of adjacency matrices. *Journal of Mathematical Chemistry*, 18(2):115–119, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164652`.

deGiambiagi:1995:ACD

[463] Myriam M. S. de Giambiagi, Mario Giambiagi, and André Ricardo Fonseca. About a certain dynamical system in molecular configuration space. *Journal of Mathematical Chemistry*, 18(2):121–132, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164653`.

Mezey:1995:RCAb

[464] Paul G. Mezey. Rules on chiral and achiral molecular transformations. II. *Journal of Mathematical Chemistry*, 18(2):133–139, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164654`.

Mezey:1995:MDM

[465] Paul G. Mezey. Macromolecular density matrices and electron densities with adjustable nuclear geometries. *Journal of Mathematical Chemistry*, 18(2):141–168, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164655`.

Arimoto:1995:NAL

[466] Shigeru Arimoto, Mark Spivakovsky, and Keith F. Taylor. Notes on the asymptotic linearity theorems. *Journal of Mathematical Chemistry*, 18(2):169–177, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164656`.

Bespalova:1995:PJM

[467] S. V. Bespalova and K. B. Tolpygo. On the problem of joint motion of interacting quantum and classical systems in the process of excitation transfer in a quantum subsystem. *Journal of Mathematical Chemistry*, 18(2):179–195, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164657`.

Fernandez:1995:EPR

[468] Francisco M. Fernández. Energy of a perturbed rigid rotor. *Journal of Mathematical Chemistry*, 18(2):197–208, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164658`.

Smeyers:1995:NRG

[469] Yves G. Smeyers, Maria Villa, and Elba Ortiz. The non-rigid group for wagging and torsion modes in methvlamine. *Journal of Mathematical Chemistry*, 18(2):209–216, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164659`.

Bracken:1995:ACS

[470] P. Bracken and J. Cízek. Analytic calculation of second-order perturbatior energy for the one-dimensional Hubbard model in the Hückel limit. *Journal of Mathematical Chemistry*, 18(2):217–235, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164660`.

Carbo:1995:QMS

[471] R. Carbó, E. Besalú, Ll. Amat, and X. Fradera. Quantum molecular similarity measures (QMSM) as a natural way leading towards a theoretical foundation of quantitative structure-properties relationships (QSPR). *Journal of Mathematical Chemistry*, 18(2):237–246, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164661`.

Amann:1995:SDS

[472] Anton Amann. Structure, dynamics and spectroscopy of single molecules: A challenge to quantum mechanics. *Journal of Mathematical Chemistry*, 18(2):247–308, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164662`.

Morales:1995:KPA

[473] J. Morales, G. Arreaga, J. J. Peña, V. Gaftoi, and G. Ovando. Kratzer potential algebraic representation and matrix elements recurrence formulae. *Journal of Mathematical Chemistry*, 18(2):309–320, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164663`.

Klein:1995:SDP

[474] D. J. Klein. Similarity and dissimilarity in posets. *Journal of Mathematical Chemistry*, 18(2):321–348, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164664`.

Aquino:1995:ASQ

[475] N. Aquino. Asymptotic series for the quantum quartic anharmonic oscillator. *Journal of Mathematical Chemistry*, 18(2):349–357, September 1995. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01164665`.

Ellzey:1996:EIT

[476] M. L. Ellzey, Jr. Elements of irreducible tensorial matrices generated by finite groups with applications to ligand field Hamiltonians. *Journal of Mathematical Chemistry*, 19(1):1–13, October 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165126`.

Merkin:1996:ABF

[477] J. H. Merkin, A. J. Poole, S. K. Scott, J. D. B. Smith, and B. W. Thompson. Analysis of the bromate-ferroin clock reaction. *Journal of Mathematical Chemistry*, 19(1):15–32, October 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165127`.

Pogliani:1996:GTP

[478] Lionello Pogliani, Giuseppe Ranieri, and Luigi Coppola. The geometry of thermodynamic potentials. *Journal of Mathematical Chemistry*, 19 (1):33–41, October 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165128`.

Blinder:1996:CPF

[479] S. M. Blinder. Canonical partition function for the hydrogen atom in curved space. *Journal of Mathematical Chemistry*, 19(1):43–46, October 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165129`.

Carbo:1996:QMS

[480] R. Carbó, E. Besalú, Ll. Amat, and X. Fradera. On quantum molecular similarity measures (QMSM) and indices (QMSI). *Journal of Mathematical Chemistry*, 19(1):47–56, October 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165130`.

Bracken:1996:NTI

[481] P. Bracken. Numerical techniques for investigating an excited state of the anisotropic Heisenberg model. *Journal of Mathematical Chemistry*, 19(1):57–74, October 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165131`.

Witwit:1996:ELS

[482] M. R. M. Witwit. The energy levels for a symmetric and nonsymmetric double-well potential in a two-dimensional system using the Hill determinant approach. *Journal of Mathematical Chemistry*, 19(1): 75–86, October 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165132`.

Baldridge:1996:PIS

[483] Kim K. Baldridge. Parallel implementation of semiempirical quantum methods for the Intel platforms. *Journal of Mathematical Chemistry*, 19 (1):87–109, October 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165133`.

Wilhelm:1996:MAS

[484] Thomas Wilhelm and Reinhart Heinrich. Mathematical analysis of the smallest chemical reaction system with Hopf bifurcation. *Journal of Mathematical Chemistry*, 19(2):111–130, June 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165179`.

Lai:1996:CFW

[485] Shan-Tao Lai, P. Palting, and Ying-Nan Chiu. On the closed form of Wigner rotation matrix elements. *Journal of Mathematical Chemistry*, 19(2):131–145, June 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165180`.

Chauvin:1996:EDC

[486] Remi Chauvin. Entropy in dissimilarity and chirality measures. *Journal of Mathematical Chemistry*, 19(2):147–174, June 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165181`.

delaSelva:1996:SMM

[487] Sara M. T. de la Selva, Eduardo Piña, and L. S. Garcia-Colin. On the simple Michaelis–Menten mechanism for chemical reactions. *Journal of Mathematical Chemistry*, 19(2):175–191, June 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165182`.

Gutman:1996:MFH

[488] I. Gutman and I. Nagypál. Mathematical foundation of the Hessian response equilibrium concept. *Journal of Mathematical Chemistry*, 19 (2):193–203, June 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165183`.

Znojil:1996:JPB

[489] Miloslav Znojil. Jacobi polynomials and bound states. *Journal of Mathematical Chemistry*, 19(2):205–213, June 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165184`.

Mezey:1996:RCA

[490] Paul G. Mezey. Rules on chiral and achiral molecular transformations. II. *Journal of Mathematical Chemistry*, 19(2):215, June 1996. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/BF01165185; http://link.springer.com/article/10.1007/BF01165185.

Bracken:1996:QGQ

[491] Paul Bracken. The quantum group $SU_q(2)$, quasitriangularity, and application to the q-rotator model. *Journal of Mathematical Chemistry*, 19(3): 217–230, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166715.

Aihara:1996:NSR

[492] Jun ichi Aihara and Tsuguhiro Tamaribuchi. Non-superaromatic reference for carbon nanotube as a quasi-one-dimensional π-bonding model for graphite. *Journal of Mathematical Chemistry*, 19(3):231–239, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166716.

Liang:1996:SCL

[493] Chengzhi Liang, Corinne Cerf, and Kurt Mislow. Specification of chirality for links and knots. *Journal of Mathematical Chemistry*, 19(3): 241–263, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166717.

Ponec:1996:SACa

[494] Robert Ponec, Gleb Yuzhakov, and Jaroslav Pecka. Similarity approach to chemical reactivity. Theoretical justification of the Hammond postulate. *Journal of Mathematical Chemistry*, 19(3):265–270, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166718.

Merkin:1996:CFI

[495] J. H. Merkin, A. J. Poole, and S. K. Scott. Chemical front initiation and propagation in the bromate-ferroin reaction. *Journal of Mathematical Chemistry*, 19(3):271–287, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166719.

Avery:1996:RCH

[496] John Avery and Frank Antonsen. Representation of cusps in a hyperspherical basis set. *Journal of Mathematical Chemistry*, 19(3):289–

300, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166720.

Simon:1996:GTT

[497] Peter L. Simon and Henrik Farkas. Geometric theory of trigger waves — a dynamical system approach. *Journal of Mathematical Chemistry*, 19(3): 301–315, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166721.

Ming:1996:EFD

[498] Li Ming and Chen Wenjian. The effect of Fe-doping on superconductivity of $YBa_2Cu_3O_y$. *Journal of Mathematical Chemistry*, 19(3):317–329, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166722.

Cendra:1996:GFP

[499] Hernán Cendra, Ariel Fernández, and Walter Reartes. A geometric framework for polymer folding. *Journal of Mathematical Chemistry*, 19(3):331–336, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166723.

Demiralp:1996:ULB

[500] Metin Demiralp and Herschel Rabitz. Upper and lower bounds on the control field and the quality of achieved optimally controlled quantum molecular motion. *Journal of Mathematical Chemistry*, 19(3):337–352, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166724.

Bowden:1996:SARa

[501] G. J. Bowden and T. Heseltine. Some analytical results for ABC, ABCD, and XBCD coupled spin 1/2 systems. I. *Journal of Mathematical Chemistry*, 19(3):353–364, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01166725.

Bowden:1996:SARb

[502] G. J. Bowden, T. Heseltine, and M. J. Prandolini. Some analytical results for ABC, ABCD, and XBCD coupled spin 1/2 systems. II. *Journal*

of Mathematical Chemistry, 19(3):365–374, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166726`.

Randic:1996:MBP

[503] Milan Randić. Molecular bonding profiles. *Journal of Mathematical Chemistry*, 19(3):375–392, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166727`.

Kolossvary:1996:ITE

[504] István Kolossváry. Information theory and electron density. *Journal of Mathematical Chemistry*, 19(3):393–399, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166728`.

Bartell:1996:LRD

[505] Lawrence S. Bartell. On the limiting radial distribution function for hydrogenic orbitals. *Journal of Mathematical Chemistry*, 19(3):401–403, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01166729`.

Stadler:1996:LTC

[506] Peter F. Stadler. Landscapes and their correlation functions. *Journal of Mathematical Chemistry*, 20(1):1–45, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165154`.

Ober:1996:STF

[507] Raimund J. Ober and E. Sally Ward. A system theoretic formulation of NMR experiments. *Journal of Mathematical Chemistry*, 20(1):47–65, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165155`.

Narumi:1996:EPM

[508] Hideyuki Narumi, Hideaki Kita, and Haruo Hosoya. Expressions for the perfect matching numbers of cubic $l \times m \times n$ lattices and their asymptotic values. *Journal of Mathematical Chemistry*, 20(1):67–77, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165156`.

Randic:1996:HOF

[509] Milan Randić, Daniel A. Morales, and Oswaldo Araujo. Higher-order Fibonacci numbers. *Journal of Mathematical Chemistry*, 20(1): 79–94, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165157`.

Fernandez:1996:APB

[510] Ariel Fernández and Gustavo Appignanesi. An action principle for biopolymer folding in vitro: A new perspective on the design of expeditiously-folded RNA molecules. *Journal of Mathematical Chemistry*, 20(1):95–116, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165158`.

Hoffman:1996:VDE

[511] D. K. Hoffman, T. L. Marchioro II, Mark Arnold, Youhong Huang, Wei Zhu, and Donald J. Kouri. Variational derivation and extensions of distributed approximating functionals. *Journal of Mathematical Chemistry*, 20(1):117–140, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165159`.

Hollauer:1996:PSM

[512] Eduardo Hollauer. The permutational symmetry in matrix multiplications. *Journal of Mathematical Chemistry*, 20(1):141–149, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165160`.

Molina:1996:ASPa

[513] A. Molina, J. González, C. Serna, and F. Balibrea. Application of the superposition principle to the study of multistep electrode processes and systems with several components in chronopotentiometry with programmed current. Part I. *Journal of Mathematical Chemistry*, 20(1): 151–167, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165161`.

Molina:1996:ASPb

[514] A. Molina, J. González, C. Serna, and L. Camacho. Application of the superposition principle to the study of a charge transfer reaction in cyclic chronopotentiometry. Part II. *Journal of Mathematical Chemistry*, 20

(1):169–181, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165162.

Jyoti:1996:IFE

[515] A. Jyoti, P. Chen, and A. W. Neumann. Invariance of free energy against a shift of the dividing surface of arbitrary geometry. *Journal of Mathematical Chemistry*, 20(1):183–192, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165163.

Pogliani:1996:MCM

[516] Lionello Pogliani, Mário N. Berberan-Santos, and José M. G. Martinho. Matrix and convolution methods in chemical kinetics. *Journal of Mathematical Chemistry*, 20(1):193–210, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165164.

Wang:1996:ASN

[517] Jianji Wang, Shiming Cao, and Ying Li. An algebraic solution for the numbers of staggered conformers of alkanes. *Journal of Mathematical Chemistry*, 20(1):211–212, March 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/BF01165165; http://link.springer.com/article/10.1007/BF01165165.

Sadiq:1996:TWO

[518] M. A. Sadiq and J. H. Merkin. Travelling waves in an open cubic autocatalytic system. *Journal of Mathematical Chemistry*, 20(2):213–233, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165344.

Taseli:1996:ASS

[519] H. Taseli. An alternative series solution to the isotropic quartic oscillator in N dimensions. *Journal of Mathematical Chemistry*, 20(2):235–245, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/BF01165345.

Carbo-Dorca:1996:EMS

[520] Ramon Carbó-Dorca and Emili Besalú. Extending molecular similarity to energy surfaces: Boltzmann similarity measures and indices. *Journal*

of Mathematical Chemistry, 20(2):247–261, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165346`.

Carbo-Dorca:1996:POA

[521] Ramon Carbó-Dorca and Emili Besalú. A procedure to obtain an accurate approximation to a full CI wavefunction. *Journal of Mathematical Chemistry*, 20(2):263–271, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165347`.

Witwit:1996:AHD

[522] M. R. M. Witwit. Application of the Hill determinant approach to several forms of potentials in two- and three-dimensional quantum systems. *Journal of Mathematical Chemistry*, 20(2):273–283, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165348`.

Bowden:1996:SARc

[523] G. J. Bowden, T. Heseltine, and M. J. Prandolini. Some analytical results for spin 1/2 spin systems. III: The benzene ring. *Journal of Mathematical Chemistry*, 20(2):285–299, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165349`.

Ponec:1996:SACb

[524] Robert Ponec, Gleb Yuzhakov, and Jaroslav Pecka. Similarity approach to chemical reactivity. Torquoselectivity in pericyclic reactions. *Journal of Mathematical Chemistry*, 20(2):301–310, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165350`.

Temme:1996:DPM

[525] F. P. Temme. Determinable partitional modelling of Cayleyan SU($m \leq n/2$) $\times S_n \downarrow \mathcal{GNMR}$ spin symmetries of isotopomeric cage-clusters: Specific $S_n \geq 12 \supset \ldots \supset D_3$ group chains, for S_n-modules in high-n weak-branching limit. *Journal of Mathematical Chemistry*, 20(2):311–329, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165351`.

Soldan:1996:EMS

[526] Pavel Soldán. Extended molecular symmetry groups. *Journal of Mathematical Chemistry*, 20(2):331–349, September 1996. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165352`.

Kuhler:1996:NQF

[527] Kathleen Kuhler and Mark R. Hoffmann. A nondiagonal quasidegenerate fourth-order perturbation theory. *Journal of Mathematical Chemistry*, 20(2):351–364, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165353`.

Fishtik:1996:JTC

[528] Ilie Fishtik, Dan Geanâ, Ivan Gutman, and István Nagypál. Joule–Thomson coefficient in systems with multiple chemical equilibria. *Journal of Mathematical Chemistry*, 20(2):365–384, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165354`.

Cruz:1996:CAM

[529] R. Cruz, G. Rojas, M. Quintero, and N. López. Cluster analysis from molecular similarity matrices using a non-linear neural network. *Journal of Mathematical Chemistry*, 20(2):385–394, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165355`.

Jayaram:1996:ARM

[530] B. Jayaram. On the acceptance ratio in Monte Carlo computer simulations. *Journal of Mathematical Chemistry*, 20(2):395–397, September 1996. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/BF01165356`.

Defranceschi:1997:CMM

[531] M. Defranceschi and C. Le Bris. Computing a molecule: A mathematical viewpoint. *Journal of Mathematical Chemistry*, 21(1):1–30, June 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019197613932`.

Palting:1997:HOT

[532] Pancracio Palting, Shan Tao Lai, Ying Nan Chiu, and Jorge Ricardo Letelier. Harmonic oscillator tensors. III: Efficient algorithms for evaluating matrix elements of vibrational operators. *Journal of Mathematical*

Chemistry, 21(1):31–49, June 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019101914841`.

Piecuch:1997:CEE

[533] Piotr Piecuch and Josef Paldus. The convergence of energy expansions for molecules in electrostatic fields: A linear-response coupled-cluster study. *Journal of Mathematical Chemistry*, 21(1):51–70, June 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019110116658`.

Kier:1997:CAM

[534] Lemont B. Kier and Chao-Kun Cheng. A cellular automata model of the soluble state. *Journal of Mathematical Chemistry*, 21(1):71–81, June 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019106015749`.

Huillet:1997:CAB

[535] Thierry Huillet and Bernard Jeannet. A combinatorial approach to branched polymers' statistics. *Journal of Mathematical Chemistry*, 21 (1):83–101, June 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019158032588`.

Roy:1997:CNC

[536] Tapon Roy. Calibrated nonparametric confidence sets. *Journal of Mathematical Chemistry*, 21(1):103–109, June 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019153931679`.

Taneri:1997:BAT

[537] Ufuk Taneri. On the bifurcation analysis of a three-dimensional non-autonomous model of molecular systems. *Journal of Mathematical Chemistry*, 21(1):111–113, June 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019149730770`.

Hoffman:1997:RPF

[538] Gary G. Hoffman. The rotational partition function for linear molecules. *Journal of Mathematical Chemistry*, 21(2):115–129, July 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019162100728`.

Farinha:1997:NLL

[539] J. P. S. Farinha, J. M. G. Martinho, and Lionello Pogliani. Non-linear least-squares and chemical kinetics. An improved method to analyse monomer-excimer decay data. *Journal of Mathematical Chemistry*, 21 (2):131–139, July 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019114217567`.

Wieland:1997:CCC

[540] Thomas Wieland. Combinatorics of combinatorial chemistry. *Journal of Mathematical Chemistry*, 21(2):141–157, July 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019166201637`.

Liu:1997:GSB

[541] Jing-Yao Liu, Chia-Chung Sun, Xu-Ri Huang, and Ze-Sheng Li. On geminals and symplectic bases in quantum chemistry. *Journal of Mathematical Chemistry*, 21(2):159–182, July 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019118318475`.

Panja:1997:GPC

[542] M. M. Panja and B. Talukdar. Geometric phase from a combined evolution-operator-invariant technique. *Journal of Mathematical Chemistry*, 21(2):183–192, July 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019170302545`.

Brunvoll:1997:ETL

[543] J. Brunvoll, S. J. Cyvin, and B. N. Cyvin. Enumeration of tree-like octagonal systems. *Journal of Mathematical Chemistry*, 21(2):193–196, July 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019122419384`.

Mackay:1997:RH

[544] Alan L. Mackay. On the regular heptagon. *Journal of Mathematical Chemistry*, 21(2):197–209, July 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019174403454`.

delaVega:1997:TCS

[545] J. M. García de la Vega, B. Miguel, and G. Ramírez. Two-center p-space integrals: diatomic molecular moments. *Journal of Mathematical Chemistry*, 21(2):211–222, July 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019126520292`.

Najfeld:1997:ERS

[546] Igor Najfeld and Timothy F. Havel. Embedding with a rigid substructure. *Journal of Mathematical Chemistry*, 21(3):223–260, October 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019190907089`.

Klein:1997:FSF

[547] D. J. Klein, N. H. March, and A. K. Theophilou. Form of spinless first- and second-order density matrices in atoms and molecules, derived from eigenfunctions of S^2 and S_z. *Journal of Mathematical Chemistry*, 21 (3):261–272, October 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019178504363`.

Morales:1997:AAC

[548] J. Morales, J. J. Peña, G. Ovando, and V. Gaftoi. Algebraic approach to closed formulation of Kratzer potential integrals. *Journal of Mathematical Chemistry*, 21(3):273–283, October 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019130621201`.

Avery:1997:MPS

[549] John Avery. Many-particle Sturmians. *Journal of Mathematical Chemistry*, 21(3):285–304, October 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019182705271`.

Finlayson:1997:TWO

[550] A. B. Finlayson and J. H. Merkin. Travelling waves in an open quadratic autocatalytic chemical system. *Journal of Mathematical Chemistry*, 21 (3):305–321, October 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019134822110`.

Ponec:1997:EPC

[551] Robert Ponec. Electron pairing and chemical bonds. Chemical structure, valences and structural similarities from the analysis of the Fermi holes. *Journal of Mathematical Chemistry*, 21(3):323–333, October 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019186806180`.

Temme:1997:BRB

[552] Francis Temme. Book review: *Group Theory and Physics* by S. Sternberg; published by Cambridge University Press. *Journal of Mathematical Chemistry*, 21(3):335–337, October 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019138923018`.

Max:1997:BEH

[553] J.-J. Max, A. F. Antippa, and C. Chapados. Boundary effects in the hexagonal packing of rod-like molecules inside a right circular cylindrical domain. I. The case of right circular spherocylindrical molecules. *Journal of Mathematical Chemistry*, 21(4):339–358, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019195007997`.

Simos:1997:EOM

[554] T. E. Simos. Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem. *Journal of Mathematical Chemistry*, 21(4):359–372, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019147124835`.

Temme:1997:SCD

[555] F. P. Temme. Some conjectures on S_n-derived nuclear permutational (or NMR) spin encodings. *Journal of Mathematical Chemistry*, 21(4):373–384, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019199108906`.

Roussel:1997:FCI

[556] Marc R. Roussel. Forced-convergence iterative schemes for the approximation of invariant manifolds. *Journal of Mathematical Chemistry*, 21(4):385–393, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019151225744`.

Besalu:1997:IMS

[557] Emili Besalú and Ramon Carbó-Dorca. An iterative method to solve the algebraic eigenvalue problem. *Journal of Mathematical Chemistry*, 21(4): 395–412, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019103309814`.

Sobaszek:1997:ITC

[558] A. Sobaszek and L. Adamowicz. The influence of the transmission coefficient of the boundary on the diffusion in a solid surrounded by vacuum. *Journal of Mathematical Chemistry*, 21(4):413–434, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019143023927`.

Ober:1997:CAM

[559] Raimund J. Ober and E. Sally Ward. On the class of attainable multidimensional NMR spectra. *Journal of Mathematical Chemistry*, 22 (1):1–10, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019167729379`.

Witwit:1997:IPP

[560] M. R. M. Witwit. Inner product perturbation theory: Energy levels of double-well potentials for two-dimensional quantum systems by expanding the potential functions around their minima. *Journal of Mathematical Chemistry*, 22(1):11–23, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019115712540`.

Reynolds:1997:CCP

[561] David Reynolds, Anthony J. Mulholland, and Jagannathan Gomatam. Calculation of chemical and phase equilibria via simulated annealing. *Journal of Mathematical Chemistry*, 22(1):25–37, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019163628470`.

Szili:1997:OTI

[562] L. Szili and J. Tóth. On the origin of Turing instability. *Journal of Mathematical Chemistry*, 22(1):39–53, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019159427561`.

Jingjiang:1997:MRT

[563] Liu Jingjiang, Liu Fengying, and Wang Yi. Modified rotation transformation method for the calculation of repulsion integrals. *Journal of Mathematical Chemistry*, 22(1):55–84, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019155326653`.

Besalu:1997:RSP

[564] Emili Besalú and Ramon Carbó-Dorca. Rayleigh–Schrödinger perturbation theory: Practical implementation of matrix and vector formalisms and description of an heuristic sufficiency convergence criterion. *Journal of Mathematical Chemistry*, 22(1):85–95, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019107410723`.

dePadua:1997:GCS

[565] Antonio de Pádua, J. A. de Miranda-Neto, Isaac M. Xavier, Jr., and Fernando Moraes. On the geometry and conformation of starburst dendrimers. *Journal of Mathematical Chemistry*, 22(1):97–106, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019111511632`.

Lograd o:1997:PTP

[566] P. G. Lograd o and J. D. M. Vianna. Partitioning technique procedure revisited: Formalism and first application to atomic problems. *Journal of Mathematical Chemistry*, 22(2–4):107–116, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019119813449`.

Brewster:1997:WES

[567] M. E. Brewster, George I. Fann, and Zhiyun Yang. Wavelets for electronic structure calculations. *Journal of Mathematical Chemistry*, 22(2–4):117–142, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019171830287`.

Carbo-Dorca:1997:FSB

[568] Ramon Carbó-Dorca. Fuzzy sets and Boolean tagged sets. *Journal of Mathematical Chemistry*, 22(2–4):143–147, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019123914357`.

Tellez:1997:MP

[569] Manuel Aguirre Téllez. The multiplicative product $(\delta(x_0-|x|)/\,|x|^{(n-2)/2})(\delta(x_0+|x|)/\,|x|^{(n-2)/2})$. *Journal of Mathematical Chemistry*, 22(2–4):149–160, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019128015266`.

Gadomski:1997:DKM

[570] Adam Gadomski. Description of the kinetics of a model tribopolymerization process. *Journal of Mathematical Chemistry*, 22(2–4):161–183, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019180032104`.

Petitjean:1997:ASK

[571] Michel Petitjean. About second kind continuous chirality measures. 1. Planar sets. *Journal of Mathematical Chemistry*, 22(2–4):185–201, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019132116175`.

Plakhutin:1997:CCS

[572] Boris N. Plakhutin. Coupling coefficients "symmetry dilemma" in the restricted open-shell Hartree–Fock method. *Journal of Mathematical Chemistry*, 22(2–4):203–233, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019184100245`.

Rerat:1997:TPH

[573] Michel Rérat, Michel Gélize, and Daniel Liotard. Topology of potential hypersurfaces of two, three and four dipoles interacting at long distances. *Journal of Mathematical Chemistry*, 22(2–4):235–247, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019136217083`.

Friis-Jensen:1997:NPS

[574] Britt Friis-Jensen, David L. Cooper, and Sten Rettrup. Normalization of projected spin eigenfunctions. *Journal of Mathematical Chemistry*, 22(2–4):249–254, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019175931196`.

Morales:1997:PET

[575] Daniel A. Morales. A proof of the equivalence of two formulas for the matrix elements of the Morse potential. *Journal of Mathematical Chemistry*, 22(2–4):255–257, December 1997. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019188201154`.

Mezey:1998:EF

[576] Paul G. Mezey. Editorial foreword. *Journal of Mathematical Chemistry*, 23(1–2):1, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1023/A:1019140317992`.

Woolley:1998:TQD

[577] R. G. Woolley. Is there a quantum definition of a molecule? *Journal of Mathematical Chemistry*, 23(1–2):3–12, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019144518901`.

Pinto:1998:PCE

[578] Yariv Pinto, Yair Salomon, and David Avnir. Properties and classification of enantiomerization pathways. *Journal of Mathematical Chemistry*, 23(1–2):13–29, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019148619809`.

Flapan:1998:TRG

[579] Erica Flapan. Topological rubber gloves. *Journal of Mathematical Chemistry*, 23(1–2):31–49, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019113006605`.

Allan:1998:QMS

[580] Neil L. Allan and David L. Cooper. Quantum molecular similarity via momentum-space indices. *Journal of Mathematical Chemistry*, 23 (1–2):51–60, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019165023444`.

Cassam-Chenai:1998:MDM

[581] P. Cassam-Chenaï. A mathematical definition of molecular structure — open problem. *Journal of Mathematical Chemistry*, 23(1–2):61–63,

April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019156821626`.

Mezey:1998:GCS

[582] Paul G. Mezey. Generalized chirality and symmetry deficiency. *Journal of Mathematical Chemistry*, 23(1–2):65–84, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019121208423`.

Ponec:1998:EPC

[583] Robert Ponec. Electron pairing and chemical bonds. Molecular structure from the analysis of pair densities and related quantities. *Journal of Mathematical Chemistry*, 23(1–2):85–103, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019160922535`.

Thorsteinsson:1998:NWM

[584] Thorstein Thorsteinsson and David L. Cooper. Nonorthogonal weights of modern VB wavefunctions. Implementation and applications within CASVB. *Journal of Mathematical Chemistry*, 23(1–2):105–106, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1023/A:1019100703879`.

Karwowski:1998:SGB

[585] Jacek Karwowski. Symmetric-group-based methods in quantum chemistry. *Journal of Mathematical Chemistry*, 23(1–2):127–149, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019196502971`.

Kirby:1998:ATG

[586] E. C. Kirby and Tomaz Pisanski. Aspects of topology, genus and isomerism in closed 3-valent networks. *Journal of Mathematical Chemistry*, 23(1–2):151–167, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019104804788`.

Hosoya:1998:PTN

[587] Haruo Hosoya. Pascal's triangle, non-adjacent numbers, and D-dimensional atomic orbitals. *Journal of Mathematical Chemistry*, 23 (1–2):169–178, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019192302062`.

Klein:1998:DVG

[588] D. J. Klein and H.-Y. Zhu. Distances and volumina for graphs. *Journal of Mathematical Chemistry*, 23(1–2):179–195, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019108905697`.

King:1998:SAS

[589] R. B. King. Some aspects of the symmetry and topology of possible carbon allotrope structures. *Journal of Mathematical Chemistry*, 23(1–2):197–227, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019117107514`.

Perez:1998:GPB

[590] Juan J. Perez, Marta Filizola, and Maria Caritenì-Farina. A general procedure for building the transmembrane domains of G-protein coupled receptors. *Journal of Mathematical Chemistry*, 23(1–2):229–238, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019169124352`.

Vives:1998:PFR

[591] D. Vives, J. Armero, A. Martí, L. Ramírez-Piscina, J. Casademunt, J. M. Sancho, and F. Sagués. Propagating fronts in reaction-diffusion systems. *Journal of Mathematical Chemistry*, 23(1–2):239–260, April 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019152720718`.

Redmond:1998:SHA

[592] David B. Redmond, Charles M. Quinn, and Patrick W. Fowler. A symmetrized Hückel analysis of carbon cages of I_h point group symmetry. *Journal of Mathematical Chemistry*, 23(3–4):263–276, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019125409331`.

Molina:1998:ASP

[593] A. Molina, J. González, and M. López-Tenés. Application of the superposition principle to the study of CEC, CE, EC and catalytic mechanisms in cyclic chronopotentiometry. Part III. *Journal of Mathematical Chemistry*, 23(3–4):277–296, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019173225261`.

Singh:1998:MTT

[594] Tejwant Singh, Rajinder Pal Singh, and Jatinder Dutt. Mass transfer to tubular electrodes. Part 2: CE process. *Journal of Mathematical Chemistry*, 23(3–4):297–308, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019181527078`.

Cances:1998:NAI

[595] Eric Cancès and Benedetta Mennucci. New applications of integral equations methods for solvation continuum models: ionic solutions and liquid crystals. *Journal of Mathematical Chemistry*, 23(3–4):309–326, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019133611148`.

Robert:1998:EQS

[596] David Robert and Ramon Carbó-Dorca. On the extension of quantum similarity to atomic nuclei: Nuclear quantum similarity. *Journal of Mathematical Chemistry*, 23(3–4):327–351, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019177426169`.

Carbo-Dorca:1998:TSC

[597] Ramon Carbó-Dorca. Tagged sets, convex sets and quantum similarity measures. *Journal of Mathematical Chemistry*, 23(3–4):353–364, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019185627987`.

Carbo-Dorca:1998:SID

[598] Ramon Carbó-Dorca. On the statistical interpretation of density functions: Atomic shell approximation, convex sets, discrete quantum chemical molecular representations, diagonal vector spaces and related problems. *Journal of Mathematical Chemistry*, 23(3–4):365–375, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019189728895`.

Whitley:1998:VWS

[599] David C. Whitley. Van der Waals surface graphs and molecular shape. *Journal of Mathematical Chemistry*, 23(3–4):377–397, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019137712057`.

Piris:1998:AGI

[600] Mario Piris. Analytic gradients in the improved BCS method. *Journal of Mathematical Chemistry*, 23(3–4):399–404, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019141812966`.

Sarasola:1998:CFA

[601] C. Sarasola, J. M. Elorza, and J. M. Ugalde. Closed-form analytical solutions for the calculation of the moments of the molecular electron density. *Journal of Mathematical Chemistry*, 23(3–4):405–414, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019145913874`.

Tarnai:1998:NPG

[602] Tibor Tarnai. Note on packings in Grassmannian space $G(3,1)$. *Journal of Mathematical Chemistry*, 23(3–4):415–419, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019193829804`.

Lam:1998:MRB

[603] Ching-Wan Lam. A mathematical relationship between the number of isomers of alkenes and alkynes: a result established from the enumeration of isomers of alkenes from alkyl biradicals. *Journal of Mathematical Chemistry*, 23(3–4):421–428, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019129510240`.

LeGuennec:1998:CC

[604] Patrick Le Guennec. On the concept of chirality. *Journal of Mathematical Chemistry*, 23(3–4):429–439, June 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019197930712`.

Farkas:1998:LCR

[605] Gyula Farkas. Local controllability of reactions. *Journal of Mathematical Chemistry*, 24(1–3):1–14, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019150014783`.

Farkas:1998:LOC

[606] Gyula Farkas. On local observability of chemical systems. *Journal of Mathematical Chemistry*, 24(1–3):15–22, August 1998. CODEN JM-

CHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019158316600.

Simos:1998:SEM

[607] T. E. Simos. Some embedded modified Runge–Kutta methods for the numerical solution of some specific Schrödinger equations. *Journal of Mathematical Chemistry*, 24(1–3):23–37, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019102131621.

Hornburger:1998:DCA

[608] H. Hornburger and Geerd H. F. Diercksen. Derivation of closed analytical expressions for Rosen–Morse Franck–Condon factors. *Journal of Mathematical Chemistry*, 24(1–3):39–60, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019154115691.

Knopfmacher:1998:AIE

[609] John Knopfmacher. Asymptotic isomer enumeration in chemistry. *Journal of Mathematical Chemistry*, 24(1–3):61–69, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019106332530.

Grimaldi:1998:GMC

[610] P. Grimaldi. Global methods in classical mechanics. The Euler–Lagrange equation. *Journal of Mathematical Chemistry*, 24(1–3):71–78, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019110400670.

Antippa:1998:BEH

[611] A. F. Antippa, J.-J. Max, and C. Chapados. Boundary effects in the hexagonal packing of rod-like molecules inside a right circular cylindrical domain. II: The case of inclined spherocylindrical molecules. *Journal of Mathematical Chemistry*, 24(1–3):79–108, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019162417509.

Balinska:1998:GWV

[612] Krystyna T. Balińska, Graham R. Brightwell, and Louis V. Quintas. Graphs whose vertices are graphs with bounded degree: Distance problems. *Journal of Mathematical Chemistry*, 24(1–3):109–121, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL http://link.springer.com/article/10.1023/A:1019114501579.

Lai:1998:SIW

[613] Shan-Tao Lai, Pancracio Palting, Ying-Nan Chiu, and Harris J. Silverstone. On the summations involving Wigner rotation matrix elements. *Journal of Mathematical Chemistry*, 24(1–3):123–132, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019166518417.

Temme:1998:MMN

[614] F. P. Temme. Multicolour models of natural embedding for $\mathrm{SU}(2 \geq m \geq 4) \times \mathrm{S}_{10} \downarrow D_5$ NMR spin symmetry: Determinacy of nuclear spin weights for $(1, 12)$-car^{-11} B-boranes. *Journal of Mathematical Chemistry*, 24(1–3):133–142, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019118602488.

Temme:1998:BDR

[615] F. P. Temme. n body democratic recoupling and role of Schur Fn. products on S_n, a NMR dual-group view pertinent to coherence-transfer. *Journal of Mathematical Chemistry*, 24(1–3):143–153, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019170619326.

Simek:1998:GSP

[616] Visnja Simek and Tomislav P. Zivković. Ground-state properties of benzenoid hydrocarbons by simple bond orbital resonance theory approach. *Journal of Mathematical Chemistry*, 24(1–3):155–168, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019122703396.

Avery:1998:FAH

[617] John Avery. A formula for angular and hyperangular integration. *Journal of Mathematical Chemistry*, 24(1–3):169–174, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019174720234.

Avery:1998:RSB

[618] John Avery and Frank Antonsen. Relativistic Sturmian basis functions. *Journal of Mathematical Chemistry*, 24(1–3):175–185, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019187122960.

Huillet:1998:SA

[619] Thierry Huillet. Statistics of aggregates. *Journal of Mathematical Chemistry*, 24(1–3):187–221, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019126804305`.

Harris:1998:ECD

[620] William D. Harris. On electrostatic chiral discrimination. *Journal of Mathematical Chemistry*, 24(1–3):223–231, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019178821143`.

Ruiz:1998:PPW

[621] M. Belén Ruiz. A partially projected wave function for radicals. *Journal of Mathematical Chemistry*, 24(1–3):233–248, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019130905213`.

Witwit:1998:AIP

[622] M. R. M. Witwit. Application of the inner product technique to double-well potentials in three-dimensional quantum systems by expanding the potential functions around their minima. *Journal of Mathematical Chemistry*, 24(1–3):249–259, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019182922052`.

Korobov:1998:GPH

[623] A. Korobov. Geometrical probabilities in heterogeneous kinetics: 60 years of side by side development. *Journal of Mathematical Chemistry*, 24(1–3):261–290, August 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019135006122`.

Leung:1998:QDM

[624] Ki Leung, Bernie D. Shizgal, and Heli Chen. The Quadrature Discretization Method (QDM) in comparison with other numerical methods of solution of the Fokker–Planck equation for electron thermalization. *Journal of Mathematical Chemistry*, 24(4):291–319, December 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019139207031`.

Chen:1998:QDM

[625] Heli Chen and Bernie D. Shizgal. The Quadrature Discretization Method (QDM) in the solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 24(4):321–343, December 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019191223869`.

Randic:1998:SOB

[626] Milan Randić. On structural ordering and branching of acyclic saturated hydrocarbons. *Journal of Mathematical Chemistry*, 24(4):345–358, December 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019143307939`.

Doslic:1998:LBN

[627] Tomislav Doslić. On lower bounds of number of perfect matchings in fullerene graphs. *Journal of Mathematical Chemistry*, 24(4):359–364, December 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019195324778`.

Erle:1998:BTA

[628] Dieter Erle. A boundedness theorem with application to oscillation of autocatalytic chemical reactions. *Journal of Mathematical Chemistry*, 24(4):365–378, December 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019147408848`.

Flapan:1998:ICT

[629] Erica Flapan and Brian Forcum. Intrinsic chirality of triple-layered naphthalenophane and related graphs. *Journal of Mathematical Chemistry*, 24(4):379–388, December 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019199425686`.

Anonymous:1998:E

[630] Anonymous. Erratum. *Journal of Mathematical Chemistry*, 24(4):389, December 1998. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1023/A%3A1019151509756`.

Tang:1999:NSI

[631] Au Chin Tang, Wei Cheng, An Yong Li, and Qian Shu Li. NMR spectra of icosahedral (I_h and I) fullerenes. *Journal of Mathematical Chemistry*, 25(1):1–6, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019103626595`.

Jaworska:1999:SBH

[632] Maria Jaworska and Piotr Lodowski. Symmetry breaking in HF wave functions of $Fe(CH)_2$. *Journal of Mathematical Chemistry*, 25(1):7–21, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019155610665`.

Baraldi:1999:CIP

[633] Ivan Baraldi, Carla Fiori, and Davide Vanossi. On the cycle index of point groups. *Journal of Mathematical Chemistry*, 25(1):23–30, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019107727503`.

Szalkai:1999:HMS

[634] István Szalkai. Handling multicomponent systems in $\mathbf{R}^n$. I: Theoretical results. *Journal of Mathematical Chemistry*, 25(1):31–46, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019159711574`.

Piris:1999:GSC

[635] Mario Piris. A generalized self-consistent-field procedure in the improved BCS theory. *Journal of Mathematical Chemistry*, 25(1):47–54, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019111828412`.

Tasi:1999:QAC

[636] Gyula Tasi and Fujio Mizukami. Quantum algebraic-combinatoric study of the conformational properties of n-alkanes. I. *Journal of Mathematical Chemistry*, 25(1):55–64, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019163812482`.

Simos:1999:FPS

[637] T. E. Simos. A family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation. *Journal of Mathematical*

Chemistry, 25(1):65–84, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019115929321`.

Anglada:1999:AWI

[638] Josep Maria Anglada, Emili Besalú, Josep Maria Bofill, and Jaime Rubio. Another way to implement the Powell formula for updating Hessian matrices related to transition structures. *Journal of Mathematical Chemistry*, 25(1):85–92, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019168013391`.

Arrighini:1999:MAA

[639] G. P. Arrighini, N. Durante, and C. Guidotti. The method of Airy averaging and some useful applications. *Journal of Mathematical Chemistry*, 25(1):93–103, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019120130229`.

Evans:1999:NTL

[640] C. M. Evans and G. L. Findley. A new transformation for the Lotka–Volterra problem. *Journal of Mathematical Chemistry*, 25(1):105–110, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019172114300`.

Merkin:1999:RFI

[641] J. H. Merkin and H. Sevcíková. Reaction fronts in an ionic autocatalytic system with an applied electric field. *Journal of Mathematical Chemistry*, 25(1):111–132, March 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019124231138`.

Nitta:1999:GTA

[642] Koh hei Nitta. A graph-theoretical approach to statistics and dynamics of tree-like molecules. *Journal of Mathematical Chemistry*, 25(2–3):133–143, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019176215208`.

Li:1999:MEO

[643] Huaien Li. On minimal energy ordering of acyclic conjugated molecules. *Journal of Mathematical Chemistry*, 25(2–3):145–169, June 1999. CO-

DEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019180316117.

Tellez:1999:PDC

[644] M. Aguirre Tellez, C. G. Bollini, and M. C. Rocca. On the product of distributions with coincident point singularities. *Journal of Mathematical Chemistry*, 25(2–3):171–180, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019132400187.

Evans:1999:ASF

[645] C. M. Evans and G. L. Findley. Analytic solutions to a family of Lotka–Volterra related differential equations. *Journal of Mathematical Chemistry*, 25(2–3):181–189, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019184417025.

Vibok:1999:GFO

[646] Á. Vibók and G. J. Halász. Generalization of the fourth-order Hylleraas functional for the case of a non-Hermitian unperturbed Hamiltonian. *Journal of Mathematical Chemistry*, 25(2–3):191–195, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019136501096.

Rabitz:1999:GFH

[647] Herschel Rabitz and Ömer F. Alis. General foundations of high-dimensional model representations. *Journal of Mathematical Chemistry*, 25(2–3):197–233, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019188517934.

Hoffman:1999:VAD

[648] D. K. Hoffman, G. W. Wei, and D. J. Kouri. A variational approach to the Dirichlet–Gabor wavelet-distributed approximating functional. *Journal of Mathematical Chemistry*, 25(2–3):235–244, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019140602004.

Baronas:1999:MBB

[649] R. Baronas, F. Ivanauskas, and J. Kulys. Modelling a biosensor based on the heterogeneous microreactor. *Journal of Mathematical Chemistry*, 25 (2–3):245–252, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019192618843.

Sen:1999:NLH

[650] K. D. Sen, Emili Besalú, and Ramon Carbó-Dorca. A naive look on the Hohenberg–Kohn theorem. *Journal of Mathematical Chemistry*, 25 (2–3):253–257, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019148903821.

Safouhi:1999:NLT

[651] H. Safouhi and P. E. Hoggan. Non-linear transformations for rapid and efficient evaluation of multicenter bielectronic integrals over B functions. *Journal of Mathematical Chemistry*, 25(2–3):259–280, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019101020660.

Parthasarathy:1999:ETS

[652] P. R. Parthasarathy and S. Dharmaraja. Exact transient solutions of kinetics of first-order reactions with end effects. *Journal of Mathematical Chemistry*, 25(2–3):281–294, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019153004730.

Salomon:1999:CSM

[653] Yair Salomon and David Avnir. Continuous symmetry measures: A note in proof of the folding/unfolding method. *Journal of Mathematical Chemistry*, 25(2–3):295–308, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019144702913.

Summerfield:1999:DDT

[654] J. H. Summerfield and J. G. Loeser. Dimension-dependent two-electron Hamiltonian matrix elements. *Journal of Mathematical Chemistry*, 25 (2–3):309–315, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019196719751.

Gaggero-Sager:1999:ECT

[655] L. M. Gaggero-Sager. Exchange and correlation in the Thomas–Fermi approximation. *Journal of Mathematical Chemistry*, 25(2–3):317–320, June 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1019128332046.

Grassi:1999:DUF

[656] A. Grassi, G. M. Lombardo, and A. Raudino. Discretization of unknown functions: A new method to solve partial differential equations with mixed boundary conditions. *Journal of Mathematical Chemistry*, 25(4): 321–344, September 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019105121568`.

Iachello:1999:CES

[657] F. Iachello and A. Del Sol Mesa. A class of exactly solvable matrix models. *Journal of Mathematical Chemistry*, 25(4):345–363, September 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019109222477`.

Korobov:1999:SSR

[658] A. Korobov. Solid state reaction kinetics: Structure of the simplest rate-time curve in terms of random tessellations. *Journal of Mathematical Chemistry*, 25(4):365–382, September 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019161206547`.

Frank:1999:ADF

[659] A. Frank, R. Lemus, and F. Pérez-Bernal. Algebraic derivation of Franck–Condon overlap integrals for diatomic molecules. *Journal of Mathematical Chemistry*, 25(4):383–391, September 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019113323386`.

Toth:1999:MNN

[660] J. Tóth. Multistationarity is neither necessary nor sufficient to oscillations. *Journal of Mathematical Chemistry*, 25(4):393–397, September 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019157105639`.

Lograd:1999:PTP

[661] P. G. Lograd and J. D. M. Vianna. Partitioning technique procedure revisited II: Application to the Stark and Zeeman problems in light atoms. *Journal of Mathematical Chemistry*, 26(1–3):1–13, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019165307456`.

Ober:1999:RRO

[662] Raimund J. Ober, Viswanath Ramakrishna, and E. Sally Ward. On the role of reachability and observability in NMR experimentation. *Journal of Mathematical Chemistry*, 26(1–3):15–26, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019117424294`.

Suslov:1999:ADS

[663] S. A. Suslov and A. J. Roberts. Advection-dispersion in symmetric field-flow fractionation channels. *Journal of Mathematical Chemistry*, 26(1–3):27–46, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019169408365`.

Preece:1999:CCR

[664] S. J. Preece, J. Billingham, and A. C. King. Chemical clock reactions: The effect of precursor consumption. *Journal of Mathematical Chemistry*, 26(1–3):47–73, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019121525203`.

Anisimov:1999:IPS

[665] Victor Anisimov and Piotr Paneth. ISOEFF98. A program for studies of isotope effects using Hessian modifications. *Journal of Mathematical Chemistry*, 26(1–3):75–86, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019173509273`.

Stacho:1999:MTF

[666] László L. Stachó, Gyula Dömötör, and Miklós I. Bán. Misgivings from the theoretical foundation of the path-following procedures based on the Elber–Karplus strategy. *Journal of Mathematical Chemistry*, 26(1–3):87–94, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019125626111`.

Knopfmacher:1999:AIE

[667] John Knopfmacher and Richard Warlimont. Asymptotic isomer enumeration in chemistry. II. *Journal of Mathematical Chemistry*, 26(1–3):95–99, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019177610182`.

Ceulemans:1999:HGR

[668] A. Ceulemans, R. B. King, S. A. Bovin, K. M. Rogers, A. Troisi, and P. W. Fowler. The heptakisoctahedral group and its relevance to carbon allotropes with negative curvature. *Journal of Mathematical Chemistry*, 26(1–3):101–123, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019129827020`.

Harrison:1999:SAN

[669] Robert W. Harrison. A self-assembling neural network for modeling polymers. *Journal of Mathematical Chemistry*, 26(1–3):125–137, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019181811090`.

Szakacs:1999:PMT

[670] Zoltán Szakács and Béla Noszál. Protonation microequilibrium treatment of polybasic compounds with any possible symmetry. *Journal of Mathematical Chemistry*, 26(1–3):139–155, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019133927929`.

Znojil:1999:BSK

[671] Miloslav Znojil. Bound states in the Kratzer plus polynomial potentials and the new form of perturbation theory. *Journal of Mathematical Chemistry*, 26(1–3):157–172, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019185911999`.

Peterson:1999:DTP

[672] I. R. Peterson. The distortion and tilt parameters for a 2D Bravais lattice of rod-like molecules. *Journal of Mathematical Chemistry*, 26(1–3):173–177, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019138028837`.

Antippa:1999:TOP

[673] A. F. Antippa. Tilting operator for phospholipidic molecular domains at the liquid-gas interface. *Journal of Mathematical Chemistry*, 26(1–3):179–196, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019190012908`.

Groppi:1999:KAC

[674] M. Groppi and G. Spiga. Kinetic approach to chemical reactions and inelastic transitions in a rarefied gas. *Journal of Mathematical Chemistry*, 26(1–3):197–219, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019194113816`.

Ding:1999:ADL

[675] Shiliang Ding, Xizhang Yi, Daren Guan, Benhui Yang, and Jiazhong Sun. An application of the dynamical Lie algebraic method to energy transfer of the collinear scattering system AB+CD. *Journal of Mathematical Chemistry*, 26(1–3):221–232, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019146230655`.

Nesbet:1999:DEL

[676] R. K. Nesbet and R. Colle. Does an exact local exchange potential exist? *Journal of Mathematical Chemistry*, 26(1–3):233–242, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019198214725`.

Szmytkowski:1999:SWD

[677] Radosław Szmytkowski and Czesław Szmytkowski. Scalar wave diffraction from zero-range scatterers. *Journal of Mathematical Chemistry*, 26(1–3):243–254, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019150331563`.

Berberan-Santos:1999:TAD

[678] Mário N. Berberan-Santos and Lionello Pogliani. Two alternative derivations of Bridgman's theorem. *Journal of Mathematical Chemistry*, 26(1–3):255–261, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019102415633`.

Lipkus:1999:PTI

[679] Alan H. Lipkus. A proof of the triangle inequality for the Tanimoto distance. *Journal of Mathematical Chemistry*, 26(1–3):263–265, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019154432472`.

Temme:1999:BR

[680] F. Temme. Book reviews. *Journal of Mathematical Chemistry*, 26(1–3):267–269, October 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019142129746`.

Bokanowski:1999:NRR

[681] Olivier Bokanowski. New N-representability results with symmetry in molecular quantum chemistry. *Journal of Mathematical Chemistry*, 26(4):271–296, December 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019106516542`.

Twizell:1999:SOS

[682] E. H. Twizell, A. B. Gumel, and Q. Cao. A second-order scheme for the "Brusselator" reaction–diffusion system. *Journal of Mathematical Chemistry*, 26(4):297–316, December 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019158500612`.

Pejov:1999:PTM

[683] Ljupco Pejov and Gjorgji Ivanovski. A perturbation theoretical method for determination of the dependence of the intramolecular X–H(D) potential on the hydrogen bond strength. *Journal of Mathematical Chemistry*, 26(4):317–326, December 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019110717451`.

Avdelas:1999:EEO

[684] G. Avdelas and T. E. Simos. Embedded eighth order methods for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 26(4):327–341, December 1999. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1019162701521`.

Aguirre:2000:SMP

[685] Manuel A. Aguirre. On some multiplicative product of kth derivative of Dirac's delta in $x_0+|x|$ and $x_0-|x|$. *Journal of Mathematical Chemistry*, 27(1–2):1–12, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019114818359`.

Pecka:2000:SAM

[686] J. Pecka and R. Ponec. Simple analytical method for evaluation of statistical importance of correlations in QSAR studies. *Journal of Mathematical Chemistry*, 27(1–2):13–22, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019166802430`.

Lam:2000:EIA

[687] Ching-Wan Lam. Enumeration of isomers of alkylcyclopropanes by means of alkyl 1,1-biradicals. *Journal of Mathematical Chemistry*, 27 (1–2):23–25, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019118919268`.

Marmorino:2000:IAM

[688] M. G. Marmorino. Incompleteness of atomic and molecular eigenfunctions. *Journal of Mathematical Chemistry*, 27(1–2):27–30, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019170903338`.

Marmorino:2000:ESB

[689] M. G. Marmorino. An exactly soluble base problem for atomic systems. *Journal of Mathematical Chemistry*, 27(1–2):31–34, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019143624720`.

Carbo-Dorca:2000:DAM

[690] Ramon Carbó-Dorca. A discussion on an apparent MO theory paradox. *Journal of Mathematical Chemistry*, 27(1–2):35–41, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019123020177`.

Avery:2000:GSA

[691] John Avery and Cecilia Coletti. Generalized Sturmians applied to atoms in strong external fields. *Journal of Mathematical Chemistry*, 27(1–2):43–51, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019175004247`.

Mezey:2000:HAT

[692] Paul G. Mezey. The T-hull approach to transformations of discrete point sets to continua and shape transformations between discontinuous objects using alpha-hulls. *Journal of Mathematical Chemistry*, 27

(1–2):53–60, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019127121085`.

Mezey:2000:SSR

[693] Paul G. Mezey. Shape-similarity relations based on topological resolution. *Journal of Mathematical Chemistry*, 27(1–2):61–69, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019179105155`.

Wilhelm:2000:CSC

[694] Thomas Wilhelm. Chemical systems consisting only of elementary steps-a paradigma for nonlinear behavior. *Journal of Mathematical Chemistry*, 27(1–2):71–88, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019131221994`.

Siegel:2000:GSC

[695] D. Siegel and D. MacLean. Global stability of complex balanced mechanisms. *Journal of Mathematical Chemistry*, 27(1–2):89–110, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019183206064`.

Temme:2000:DGTa

[696] F. P. Temme. On SU(2) $\times \mathcal{S}_{\backslash \geq \infty \in}$ dual-group tensorial sets and carrier spaces in the multiple invariant physics of multiquantum NMR. I. $k > n/2$ rank maximal $\left\{ \sum_v T^k(v) \rightarrow \sum_{\tilde{\lambda}'} \Lambda_{\cdot,\tilde{\lambda}'}[\tilde{\lambda}'] \right\}$ Liouvillian $\overline{\mathrm{U}} \times \mathcal{P}$ mappings. *Journal of Mathematical Chemistry*, 27(1–2):111–130, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019135322902`.

Temme:2000:DGTb

[697] F. P. Temme. On SU(2) $\times \mathcal{S}_{\backslash \geq \infty \in}$ dual-group tensorial sets and carrier spaces in the multiple invariant physics of multiquantum NMR. II. $\{\mathcal{S}_{\infty \in} \supset \cdots \supset [\in]\mathcal{S}_{\in}\}$ pathways from Yamanouchi monomial reductions as $[A]_{12}$ democratic S_n-invariant labels. *Journal of Mathematical Chemistry*, 27(1–2):131–154, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019187306973`.

Schnell:2000:EKM

[698] S. Schnell and C. Mendoza. Enzyme kinetics of multiple alternative substrates. *Journal of Mathematical Chemistry*, 27(1–2):155–170, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019139423811`.

Saez:2000:TLC

[699] E. Sáez, I. Szántó, and A. Monsalve. Three limit cycles for a first-order exothermic chemical reaction in a continuous stirred-tank reactor. *Journal of Mathematical Chemistry*, 27(1–2):171–182, October 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1019191507881`.

Singh:2000:MTT

[700] Rajinder Pal Singh, Tejwant Singh, Jatinder Dutt, and Atamjyot. Mass transfer to tubular electrodes: ECE process. *Journal of Mathematical Chemistry*, 27(3):183–190, November 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1026420118672`.

Tasi:2000:QAC

[701] Gyula Tasi, Fujio Mizukami, and József Csontos. Quantum algebraic-combinatoric study of the conformational properties of n-alkanes. II. *Journal of Mathematical Chemistry*, 27(3):191–199, November 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1026472102742`.

Araujo:2000:RIL

[702] Oswaldo Araujo and Juan Rada. Randić index and lexicographic order. *Journal of Mathematical Chemistry*, 27(3):201–212, November 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1026424219580`.

Arimoto:2000:MMD

[703] Shigeru Arimoto. Magic mountain and Devil's staircase swapping problems. *Journal of Mathematical Chemistry*, 27(3):213–217, November 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1026476203651`.

Qian:2000:MTM

[704] Hong Qian. The mathematical theory of molecular motor movement and chemomechanical energy transduction. *Journal of Mathematical Chemistry*, 27(3):219–234, November 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1026428320489`.

Mezei:2000:NAC

[705] Mihaly Mezei. A novel approach to the calculation of the free energy due to molecular flexibility. *Journal of Mathematical Chemistry*, 27(3): 235–250, November 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1026480304559`.

Bao:2000:EES

[706] Gang Bao, Xiaohong Fang, Weihong Tan, and Tri Van. Evanescent energy in square and circular fibers. *Journal of Mathematical Chemistry*, 27(4):251–265, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018889304472`.

Baronas:2000:SEB

[707] R. Baronas, F. Ivanauskas, and A. Survila. Simulation of electrochemical behavior of partially blocked electrodes under linear potential sweep conditions. *Journal of Mathematical Chemistry*, 27(4):267–278, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018867621310`.

Avery:2000:GSM

[708] John Avery. The generalized Sturmian method and inelastic scattering of fast electrons. *Journal of Mathematical Chemistry*, 27(4):279–292, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018819705380`.

Erle:2000:NCR

[709] Dieter Erle. Nonoscillation in closed reversible chemical systems. *Journal of Mathematical Chemistry*, 27(4):293–302, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018871722219`.

Soss:2000:GCA

[710] Michael Soss and Godfried T. Toussaint. Geometric and computational aspects of polymer reconfiguration. *Journal of Mathematical Chemistry*, 27(4):303–318, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018823806289`.

Zhang:2000:EHC

[711] Lian zhu Zhang and Fu ji Zhang. Extremal hexagonal chains concerning k-matchings and k-independent sets. *Journal of Mathematical Chemistry*, 27(4):319–329, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018875823127`.

Park:2000:ETC

[712] Yung Park. Effect of transient condensation of a supercooled gas on the size distribution of new-phase particles. *Journal of Mathematical Chemistry*, 27(4):331–342, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018827907198`.

Simos:2000:NEB

[713] T. E. Simos. A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 27(4):343–356, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018879924036`.

Carbo-Dorca:2000:QQE

[714] Ramon Carbó-Dorca. Quantum QSAR and the eigensystems of stochastic quantum similarity matrices. *Journal of Mathematical Chemistry*, 27(4):357–376, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018832008106`.

Szalkai:2000:VOS

[715] István Szalkai. On valuation operators in stoichiometry and in reaction syntheses. *Journal of Mathematical Chemistry*, 27(4):377–386, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018884024945`.

Anonymous:2000:AIa

[716] Anonymous. Author index. *Journal of Mathematical Chemistry*, 27(4): 387–389, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1018842231020`.

Szalkai:2000:NGA

[717] István Szalkai. A new general algorithmic method in reaction syntheses using linear algebra. *Journal of Mathematical Chemistry*, 28(1–3): 1–34, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018836209015`.

Basu:2000:CSA

[718] Shukla Basu and R. K. Roychoudhury. The coherent state and anharmonic oscillator description of nonlinear oscillation. *Journal of Mathematical Chemistry*, 28(1–3):35–41, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018888225853`.

Merkin:2000:AED

[719] J. H. Merkin, P. L. Simon, and Z. Noszticzius. Analysis of the electrolyte diode. Electro-diffusion and chemical reaction within a hydrogel reactor. *Journal of Mathematical Chemistry*, 28(1–3):43–58, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018840309923`.

Bach:2000:QCS

[720] Albert Bach, Lluis Amat, Emili Besalú, Ramon Carbó-Dorca, and Robert Ponec. Quantum chemistry, Sobolev spaces and SCF. *Journal of Mathematical Chemistry*, 28(1–3):59–70, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018892326762`.

Bollini:2000:GLM

[721] Carlos Guido Bollini, Mario Giambiagi, Myriam Segre de Giambiagi, and Aloysio Paiva de Figueiredo. Graphical linking of a MO multicenter bond index to VB structures. *Journal of Mathematical Chemistry*, 28(1–3):71–81, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018844410832`.

Bochicchio:2000:TPA

[722] R. Bochicchio, L. Lain, A. Torre, and R. Ponec. Topological population analysis from higher order densities. I. Hartree–Fock level. *Journal of Mathematical Chemistry*, 28(1–3):83–90, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018896427670`.

Kliesch:2000:PESa

[723] Wolfgang Kliesch. Potential energy surface exploration with equilibrial paths. Part I: Theory. *Journal of Mathematical Chemistry*, 28(1–3): 91–112, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018848511741`.

Kliesch:2000:PESb

[724] Wolfgang Kliesch. Potential energy surface exploration with equilibrial paths. Part II: Application. *Journal of Mathematical Chemistry*, 28(1–3): 113–138, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018800628579`.

Znojil:2000:PMT

[725] Miloslav Znojil. Perturbation method with triangular propagators and anharmonicities of intermediate strength. *Journal of Mathematical Chemistry*, 28(1–3):139–167, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018852612649`.

Hefferlin:2000:ULE

[726] Ray Hefferlin and Jonathan Knoll. On the use of Laplace's equation for global predictions of internuclear separation and dissociation energy. *Journal of Mathematical Chemistry*, 28(1–3):169–192, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018804729488`.

Zheng:2000:PES

[727] Yujun Zheng and Shiliang Ding. Potential energy surface for linear triatomic molecules: An algebraic method. *Journal of Mathematical Chemistry*, 28(1–3):193–200, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018856713558`.

Almeida:2000:HFT

[728] Rafael Almeida, Helena Diez y Riega, and Daniel A. Morales. On the Hellmann–Feynman theorem and the corrections to the energy in the Rayleigh–Schrödinger perturbation theory. *Journal of Mathematical Chemistry*, 28(1–3):201–206, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018808830396`.

Vibok:2000:GHF

[729] Á. Vibók. Generalization of the Hylleraas functional for calculating BSSE-free intermolecular interactions: further considerations. *Journal of Mathematical Chemistry*, 28(1–3):207–212, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018860814467`.

Tan:2000:FCG

[730] Hang Tan, Muzhen Liao, Yan Wang, Guoshi Wu, and K. Balasubramanian. A flexible correlation group table (CGT) method for the relativistic configuration interaction wavefunctions. *Journal of Mathematical Chemistry*, 28(1–3):213–239, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018812931305`.

Stacho:2000:RPC

[731] László L. Stachó, Gyula Dömötör, and Miklós I. Bán. On the reaction path concept of Olender and Elber. *Journal of Mathematical Chemistry*, 28(1–3):241–246, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018875212959`.

Yang:2000:ADL

[732] Benhui Yang, Keli Han, and Shiliang Ding. Application of dynamical Lie algebraic method to atom-diatomic molecule scattering. *Journal of Mathematical Chemistry*, 28(1–3):247–266, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018878124232`.

Zivkovic:2000:VIEa

[733] Tomislav P. Zivković. Vibrational isotope effect by the low rank perturbation method. *Journal of Mathematical Chemistry*, 28(1–3):267–285, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018830208302`.

Zivkovic:2000:VIEb

[734] Tomislav P. Zivković. Vibrational isotope effect of linear and planar molecules: Deuterated bromoethenes. *Journal of Mathematical Chemistry*, 28(1–3):287–312, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018882225141`.

Pogliani:2000:CCA

[735] Lionello Pogliani and Mario N. Berberan-Santos. Constantin Carathéodory and the axiomatic thermodynamics. *Journal of Mathematical Chemistry*, 28(1–3):313–324, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1018834326958`.

Gumel:2000:NSC

[736] A. B. Gumel, W. F. Langford, E. H. Twizell, and J. Wu. Numerical solutions for a coupled non-linear oscillator. *Journal of Mathematical Chemistry*, 28(4):325–340, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1011025104111`.

Romera:2000:UBA

[737] Elvira Romera, Toshikatsu Koga, and Juan Carlos Angulo. Upper bounds to atomic electron densities in position and momentum spaces. *Journal of Mathematical Chemistry*, 28(4):341–351, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1011090920949`.

Sidhu:2000:DAE

[738] H. S. Sidhu, M. I. Nelson, G. N. Mercer, and R. O. Weber. Dynamical analysis of an elementary $X + Y \to P$ reaction in a continuously stirred tank reactor. *Journal of Mathematical Chemistry*, 28(4):353–375, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1011043005019`.

Smeyers:2000:SID

[739] Y. G. Smeyers and M. Villa. A study of the internal dynamics of trimethylamine by means of the non-rigid group theory. *Journal of Mathematical Chemistry*, 28(4):377–388, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1011095021858`.

Bungay:2000:OTS

[740] Sharene D. Bungay and Raymond A. Poirier. Optimization of transition state structures using genetic algorithms. *Journal of Mathematical Chemistry*, 28(4):389–401, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1011047105928`.

Anonymous:2000:AIb

[741] Anonymous. Author index. *Journal of Mathematical Chemistry*, 28(4): 403–405, December 2000. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A%3A1017300210461`.

Anonymous:2001:EFa

[742] Anonymous. Editorial foreword. *Journal of Mathematical Chemistry*, 29(1):1, January 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1023/A:1017306232220`.

Carbo-Dorca:2001:ESH

[743] Ramon Carbó-Dorca and Emili Besalú. Extended Sobolev and Hilbert spaces and approximate stationary solutions for electronic systems within the non-linear Schrödinger equation. *Journal of Mathematical Chemistry*, 29(1):3–20, January 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1011085616290`.

Besalu:2001:OSP

[744] Emili Besalú and Leonel Vera. On the optimal selection of principal components in QSPR studies. *Journal of Mathematical Chemistry*, 29 (1):21–34, January 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1011018900360`.

Park:2001:DPI

[745] Yung Park. Diffusion of a passive impurity through a porous media: fractal model in an unsaturated medium. *Journal of Mathematical Chemistry*, 29(1):35–40, January 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1011070917199`.

Besalu:2001:GOE

[746] E. Besalú, R. Carbó-Dorca, and J. Karwowski. Generalized one-electron spin functions and self-similarity measures. *Journal of Mathematical Chemistry*, 29(1):41–45, January 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1011023001269`.

Leherte:2001:AMA

[747] Laurence Leherte. Application of multiresolution analyses to electron density maps of small molecules: Critical point representations for molecular superposition. *Journal of Mathematical Chemistry*, 29(1):47–83, January 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1011075018107`.

Story:2001:DDO

[748] Troy Story. Dynamics on differential one-forms. *Journal of Mathematical Chemistry*, 29(2):85–96, February 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010912428750`.

Tsaune:2001:NHP

[749] A. Ya. Tsaune. Nonrelativistic Hamiltonian in the principal central moving axes for N-particle system. *Journal of Mathematical Chemistry*, 29 (2):97–125, February 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010927112820`.

Alis:2001:EIH

[750] Ömer F. Alis and Herschel Rabitz. Efficient implementation of high dimensional model representations. *Journal of Mathematical Chemistry*, 29 (2):127–142, February 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010979129659`.

Khadikar:2001:NPI

[751] Padmakar V. Khadikar, Prabhakar P. Kale, Narian V. Deshpande, Sneha Karmarkar, and Vijay K. Agrawal. Novel PI indices of hexagonal chains. *Journal of Mathematical Chemistry*, 29(2):143–150, February 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010931213729`.

Braga:2001:NCB

[752] J. P. Braga. Numerical comparison between Tikhonov regularization and singular value decomposition methods using the l curve criterion. *Journal of Mathematical Chemistry*, 29(2):151–161, February 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010983230567`.

Hou:2001:UGM

[753] Yaoping Hou. Unicyclic graphs with minimal energy. *Journal of Mathematical Chemistry*, 29(3):163–168, April 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010935321906`.

Stacho:2001:CRP

[754] L. L. Stachó, Gy. Dömötör, and M. I. Bán. "Comment" on the reply to the paper "On the Elber–Karplus Reaction Path-Following Method and Related Procedures". *Journal of Mathematical Chemistry*, 29(3):169–175, April 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010920305977`.

Aguiar:2001:FPS

[755] J. V. Aguiar and T. E. Simos. A family of P-stable eighth algebraic order methods with exponential fitting facilities. *Journal of Mathematical Chemistry*, 29(3):177–189, April 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010972322815`.

Besalu:2001:FCC

[756] Emili Besalú. Fast computation of cross-validated properties in full linear leave–many-out procedures. *Journal of Mathematical Chemistry*, 29 (3):191–204, April 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010924406885`.

Park:2001:KDC

[757] Yung Park. Kinetics on diffusion-controlled reactions in a fractal medium. *Journal of Mathematical Chemistry*, 29(3):205–211, April 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010976423724`.

Safouhi:2001:NET

[758] Hassan Safouhi. Numerical evaluation of three-center two-electron Coulomb and hybrid integrals over B functions using the HD and $H\overline{D}$ methods and convergence properties. *Journal of Mathematical Chemistry*, 29(3):213–232, April 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010994517423`.

Klein:2001:RBF

[759] D. J. Klein. Review of *Applied Finite Group Actions* by A. Kerber (Springer, Berlin, 1999). *Journal of Mathematical Chemistry*, 29(3):233–234, April 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1023/A:1010928507794`.

Jendrol:2001:MIF

[760] Stanislav Jendrol' and Marián Trenkler. More icosahedral fulleroids. *Journal of Mathematical Chemistry*, 29(4):235–243, May 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010990901493`.

Simon:2001:RBD

[761] Peter L. Simon, Elizabeth Hild, and Henrik Farkas. Relationships between the discriminant curve and other bifurcation diagrams. *Journal of Mathematical Chemistry*, 29(4):245–265, May 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010943118331`.

Sinha:2001:SAC

[762] Anjana Sinha and Nivedita Nag. SWKB approach to confined isospectral potentials. *Journal of Mathematical Chemistry*, 29(4):267–279, May 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010995102402`.

Avdelas:2001:GOGa

[763] G. Avdelas, A. Konguetsof, and T. E. Simos. A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. *Journal of Mathematical Chemistry*, 29(4):281–291, May 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010947219240`.

Avdelas:2001:GOGb

[764] G. Avdelas, A. Konguetsof, and T. E. Simos. A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator, optimization of the generator and numerical results. *Journal of Mathematical Chemistry*, 29(4):293–305, May 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1010999203310`.

Anonymous:2001:AI

[765] Anonymous. Author index. *Journal of Mathematical Chemistry*, 29 (4):307–308, May 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1023/A:1017349823783`.

Li:2001:HDM

[766] Genyuan Li, Sheng-Wei Wang, Carey Rosenthal, and Herschel Rabitz. High dimensional model representations generated from low dimensional data samples. I. mp-Cut-HDMR. *Journal of Mathematical Chemistry*, 30(1):1–30, July 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1013172329778`.

Antippa:2001:BEH

[767] A. F. Antippa, J.-J. Max, and C. Chapados. Boundary effects in the hexagonal packing of rod-like molecules inside a right circular cylindrical domain. III. The case of arbitrarily oriented spherocylindrical molecules. *Journal of Mathematical Chemistry*, 30(1):31–67, July 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1013153313849`.

Blaive:2001:MSE

[768] Bruno Blaive and Jean-Claude Ziegler. Modeling of substituent effects: Self-parametrization, a case of interdependence of the coefficients, illustrated on the linear plus cross-term models. *Journal of Mathematical Chemistry*, 30(1):69–81, July 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1013105427633`.

Wei:2001:MPD

[769] Guowei Wei, Haixiang Wang, Donald J. Kouri, Manos Papadakis, Ioannis A. Kakadiaris, and David K. Hoffman. On the mathematical properties of distributed approximating functionals. *Journal of Mathematical*

Chemistry, 30(1):83–107, July 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1013198218461`.

Pinsky:2001:CSM

[770] Mark Pinsky, Kenny B. Lipkowitz, and David Avnir. Continuous symmetry measures. VI. The relations between polyhedral point-group/subgroup symmetries. *Journal of Mathematical Chemistry*, 30(1):109–120, July 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1013133602531`.

Simos:2001:MPF

[771] T. E. Simos and Jesus Vigo Aguiar. A modified phase-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 30(1):121–131, July 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1013185619370`.

Handrock-Meyer:2001:MDD

[772] S. Handrock-Meyer, L. V. Kalachev, and K. R. Schneider. A method to determine the dimension of long-time dynamics in multi-scale systems. *Journal of Mathematical Chemistry*, 30(2):133–160, August 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1017960802671`.

Wang:2001:AFA

[773] Zheng-Wu Wang, Xi-Zhang Yi, Da-Ren Guan, and Gan-Zuo Li. An application of functional analysis method to the potential of electrical double layer for spherical micelles. *Journal of Mathematical Chemistry*, 30(2):161–167, August 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1017971619509`.

Micheletti:2001:SDS

[774] Alessandra Micheletti and Martin Burger. Stochastic and deterministic simulation of nonisothermal crystallization of polymers. *Journal of Mathematical Chemistry*, 30(2):169–193, August 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1017923703579`.

Okrasinski:2001:MEU

[775] W. Okrasiński, M. I. Parra, and F. Cuadros. Modeling evaporation using a nonlinear diffusion equation. *Journal of Mathematical Chemistry*, 30

(2):195–202, August 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1017975720418.

Fossas:2001:SMC

[776] Enric Fossas, Rosa M. Ros, and Jaume Fabregat. Sliding mode control in a bioreactor model. *Journal of Mathematical Chemistry*, 30(2): 203–218, August 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1017927804488.

Balasubramanian:2001:LVD

[777] K. Balasubramanian. Linear variational Diophantine techniques in mass balance of chemical reactions. *Journal of Mathematical Chemistry*, 30 (2):219–225, August 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1017979821326.

Carbo-Dorca:2001:IMP

[778] Ramon Carbó-Dorca. Inward matrix product algebra and calculus as tools to construct space–time frames of arbitrary dimensions. *Journal of Mathematical Chemistry*, 30(2):227–245, August 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1017931905397.

Anonymous:2001:EFb

[779] Anonymous. Editorial foreword. *Journal of Mathematical Chemistry*, 30 (3):247–248, October 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1023/A:1017433109072.

Fujita:2001:USC

[780] Shinsaku Fujita. The unit-subduced-cycle-index methods and the characteristic-monomial method. Their relationship as group-theoretical tools for chemical combinatorics. *Journal of Mathematical Chemistry*, 30 (3):249–270, October 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1015166625910.

Klein:2001:GCE

[781] D. J. Klein and O. Ivanciuc. Graph cyclicity, excess conductance, and resistance deficit. *Journal of Mathematical Chemistry*, 30(3):271–287, October 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL http://link.springer.com/article/10.1023/A:1015119609980.

Lether:2001:FAN

[782] Frank G. Lether. A family of approximations for the numerical computation of the Randles–Sevcik function in electrochemistry. *Journal of Mathematical Chemistry*, 30(3):289–297, October 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1015171626819.

Mezey:2001:HPL

[783] Paul G. Mezey. The holographic principle for latent molecular properties. *Journal of Mathematical Chemistry*, 30(3):299–303, October 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1015123710889.

Mezey:2001:UTM

[784] Paul G. Mezey. A uniqueness theorem of molecular recognition. *Journal of Mathematical Chemistry*, 30(3):305–313, October 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1015175727727.

Szekeres:2001:MPN

[785] Zsolt Szekeres and Paul G. Mezey. Mathematical problems of nuclear configuration averaging. *Journal of Mathematical Chemistry*, 30(3):315–324, October 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1015127811798.

Guo:2001:RFE

[786] Xiaofeng Guo and Milan Randić. Recursive formulae for enumeration of LM–conjugated circuits in structurally related benzenoid hydrocarbons. *Journal of Mathematical Chemistry*, 30(3):325–342, October 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1015179828636.

Zhang:2001:NLB

[787] Heping Zhang and Fuji Zhang. New lower bound on the number of perfect matchings in fullerene graphs. *Journal of Mathematical Chemistry*, 30(3):343–347, October 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1015131912706.

Zivkovic:2001:AGE

[788] Tomislav P. Zivković. Augmentation of the generalised $n \times n$ eigenvalue equation to a generalised $(n+1) \times (n+1)$ eigenvalue equation. *Journal of Mathematical Chemistry*, 30(4):349–373, November 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015183909323`.

Mezey:2001:DCR

[789] Paul G. Mezey, Peter Warburton, E. Jako, and Zsolt Szekeres. Dimension concepts and reduced dimensions in toxicological QShAR databases as tools for data quality assessment. *Journal of Mathematical Chemistry*, 30(4):375–387, November 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015138426162`.

Frolov:2001:LMM

[790] A. Frolov, E. Jako, and P. G. Mezey. Logical models of molecular shapes and their families. *Journal of Mathematical Chemistry*, 30(4): 389–409, November 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015190410232`.

Frolov:2001:MPF

[791] A. Frolov, E. Jako, and P. G. Mezey. Metric properties of factor space of molecular shapes. *Journal of Mathematical Chemistry*, 30(4):411–428, November 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015142527070`.

Cash:2001:CPR

[792] Gordon G. Cash and Jerry Ray Dias. Computation, properties and resonance topology of benzenoid monoradicals and polyradicals and the eigenvectors belonging to their zero eigenvalues. *Journal of Mathematical Chemistry*, 30(4):429–444, November 2001. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015194511140`.

Gandy:2002:NSA

[793] Paul J. F. Gandy and Jacek Klinowski. Nodal surface approximations to the zero equipotential surfaces for cubic lattices. *Journal of Mathematical Chemistry*, 31(1):1–16, January 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015444012997`.

Brown:2002:SMA

[794] E. Brown and H. Rabitz. Some mathematical and algorithmic challenges in the control of quantum dynamics phenomena. *Journal of Mathematical Chemistry*, 31(1):17–63, January 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015482329835`.

Persson:2002:MTI

[795] L. Persson, U. Cegrell, N. Usova, and P.-O. Westlund. The mathematical theory of Ito diffusions on hypersurfaces, with applications to NMR relaxation problems. *Journal of Mathematical Chemistry*, 31(1):65–89, January 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015434413906`.

Glushkov:2002:SUF

[796] V. N. Glushkov. Spin-unrestricted formalism for a partially restricted Hartree–Fock approach. *Journal of Mathematical Chemistry*, 31(1):91–103, January 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015486430744`.

Tschumper:2002:SPT

[797] Gregory S. Tschumper and Mark R. Hoffmann. Superconvergent perturbation theory for an anharmonic oscillator. *Journal of Mathematical Chemistry*, 31(1):105–120, January 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015438514814`.

Yildirim:2002:KAM

[798] Necmettin Yildirim, Mehmet Çiftçi, and Ö. Irfan Küfrevioğlu. Kinetic analysis of multi enzyme systems: A case study of the closed system of creatine kinase, hexokinase and glucose 6-phosphate dehydrogenase. *Journal of Mathematical Chemistry*, 31(1):121–130, January 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015490531653`.

Marmorino:2002:QMP

[799] M. G. Marmorino. Quantum-mechanical proof of a Redheffer inequality. *Journal of Mathematical Chemistry*, 31(1):131–133, January 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1015442715723`.

Simos:2002:SEA

[800] T. E. Simos and Jesus Vigo-Aguiar. Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 31(2):135–144, February 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1016259830419`.

Cassam-Chenai:2002:FAQ

[801] P. Cassam-Chenaï. Frequently asked questions on "Some Fundamental Problems with Zero Flux Partitioning of Electron Densities". *Journal of Mathematical Chemistry*, 31(2):145–153, February 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1016270714489`.

Nelson:2002:BPO

[802] M. I. Nelson and H. S. Sidhu. Bifurcation phenomena for an oxidation reaction in a continuously stirred tank reactor I. Adiabatic operation. *Journal of Mathematical Chemistry*, 31(2):155–186, February 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1016222831327`.

Doslic:2002:SSP

[803] Tomislav Doslić. On some structural properties of fullerene graphs. *Journal of Mathematical Chemistry*, 31(2):187–195, February 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1016274815398`.

Marmorino:2002:ETL

[804] M. G. Marmorino. Equivalence of two lower bound methods. *Journal of Mathematical Chemistry*, 31(2):197–203, February 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1016226932236`.

Marmorino:2002:ABE

[805] M. G. Marmorino. Asymptotic behavior of the t expansion. *Journal of Mathematical Chemistry*, 31(2):205–210, February 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1016279016306`.

Kalogiratou:2002:CTE

[806] Z. Kalogiratou and T. E. Simos. Construction of trigonometrically and exponentially fitted Runge–Kutta–Nyström methods for the numerical

solution of the Schrödinger equation and related problems — a method of 8th algebraic order. *Journal of Mathematical Chemistry*, 31(2):211–232, February 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1016231100377`.

Barnes:2002:NDM

[807] J. W. Barnes, S. P. Dokov, R. Acevedo, and A. Solomon. A note on distance matrices yielding elementary landscapes for the TSP. *Journal of Mathematical Chemistry*, 31(2):233–235, February 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1016283117215`.

Xu:2002:DCK

[808] Wei Guo Xu and Qian Shu Li. The dimensionlessness of chemical kinetic equation. *Journal of Mathematical Chemistry*, 31(3):237–250, April 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1020720920578`.

Maggiora:2002:GAF

[809] Gerald M. Maggiora, James D. Petke, and Jordi Mestres. A general analysis of field-based molecular similarity indices. *Journal of Mathematical Chemistry*, 31(3):251–270, April 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1020784004649`.

Wang:2002:DCB

[810] Shiying Wang. DNA computing of bipartite graphs for maximum matching. *Journal of Mathematical Chemistry*, 31(3):271–279, April 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1020808521487`.

Temme:2002:QPD

[811] F. P. Temme. Quasi-particle dual mappings on $\widetilde{\mathbf{H}}_v$ carrier spaces for dynamical structures of S_{2n}-invariant-based, integer-rank tensorial sets: A democratic-recoupling S_{2n}-compatible overview of v-auxiliary labelling in superboson algebras of uniform multispin NMR ensembles. *Journal of Mathematical Chemistry*, 31(3):281–312, April 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1020888105557`.

Simon:2002:QFPa

[812] Peter L. Simon, Serafim Kalliadasis, John H. Merkin, and Stephen K. Scott. Quenching of flame propagation with heat loss. *Journal of Mathematical Chemistry*, 31(3):313–332, April 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1020840222396`.

Lam:2002:EIA

[813] Ching-Wan Lam. Enumeration of isomers of alkylcyclobutadienes by means of alkyl 1,1,1-triradicals. *Journal of Mathematical Chemistry*, 31 (4):333–337, May 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021059703509`.

Kunze:2002:MPC

[814] Herb Kunze and David Siegel. Monotonicity properties of chemical reactions with a single initial bimolecular step. *Journal of Mathematical Chemistry*, 31(4):339–344, May 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021064420348`.

Buki:2002:RMB

[815] András Büki, Tamás Perger, Tamás Turányi, and Ulrich Maas. Repromodelling based generation of intrinsic low-dimensional manifolds. *Journal of Mathematical Chemistry*, 31(4):345–362, May 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021016504418`.

Bowden:2002:NSW

[816] G. J. Bowden. Nuclear spin-waves, multiple quantum NMR, and the benzene ring. *Journal of Mathematical Chemistry*, 31(4):363–370, May 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021068521256`.

Avdelas:2002:NPS

[817] G. Avdelas, E. Kefalidis, and T. E. Simos. New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 31 (4):371–404, May 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021020705327`.

Shiu:2002:NCK

[818] Wai Chee Shiu, Peter Che Bor Lam, Fuji Zhang, and Heping Zhang. Normal components, Kekulé patterns, and Clar patterns in plane bipartite graphs. *Journal of Mathematical Chemistry*, 31(4):405–420, May 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021072722165`.

Lim:2002:NMR

[819] Teik-Cheng Lim. A note on mathematical relationships among bond-torsion force fields. *Journal of Mathematical Chemistry*, 31(4):421–428, May 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021024806235`.

Fujita:2002:EDR

[820] Shinsaku Fujita. Enantiomeric and diastereomeric relationships of ethylene derivatives. Restructuring stereochemistry by a group-theoretical and combinatorial approach. *Journal of Mathematical Chemistry*, 32(1):1–17, July 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021287622494`.

Marmorino:2002:LBG

[821] M. G. Marmorino. Lower bounds to ground-state eigenvalues. *Journal of Mathematical Chemistry*, 32(1):19–29, July 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021211206564`.

Howard:2002:ECT

[822] I. A. Howard, N. H. March, and D. J. Klein. Edge confinement of a two-dimensional electron gas and its relevance to the electron density near a vacancy defect in graphite. *Journal of Mathematical Chemistry*, 32(1):31–37, July 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021263223403`.

Zivkovic:2002:ITF

[823] Tomislav P. Zivković. On the interaction of two finite-dimensional quantum systems. *Journal of Mathematical Chemistry*, 32(1):39–71, July 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021215307473`.

Simon:2002:QFPb

[824] Peter L. Simon, Serafim Kalliadasis, John H. Merkin, and Stephen K. Scott. Quenching of flame propagation through endothermic reaction. *Journal of Mathematical Chemistry*, 32(1):73–98, July 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021267324311`.

Zivkovic:2002:ISS

[825] Tomislav P. Zivković. Interaction of a single state with a known infinite system containing one-parameter eigenvalue band. *Journal of Mathematical Chemistry*, 32(2):99–158, August 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021219426380`.

Morimoto:2002:PTG

[826] Susumu Morimoto. A periodic table for genetic codes. *Journal of Mathematical Chemistry*, 32(2):159–200, August 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021298410450`.

Carbo-Dorca:2002:SPM

[827] Ramon Carbó-Dorca. Shell partition and metric semispaces: Minkowski norms, root scalar products, distances and cosines of arbitrary order. *Journal of Mathematical Chemistry*, 32(2):201–223, August 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021250527289`.

Baronas:2002:MDA

[828] R. Baronas, F. Ivanauskas, and J. Kulys. Modelling dynamics of amperometric biosensors in batch and flow injection analysis. *Journal of Mathematical Chemistry*, 32(2):225–237, August 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1021202611359`.

Mezey:2002:EC

[829] Paul G. Mezey. Editorial comment. *Journal of Mathematical Chemistry*, 32(3):239, October 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1023/A:1022177722361`.

Torre:2002:TPA

[830] A. Torre, L. Lain, R. Bochicchio, and R. Ponec. Topological population analysis from higher order densities II. The correlated case. *Jour-*

nal of Mathematical Chemistry, 32(3):241–248, October 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022122906431`.

Lim:2002:MRB

[831] Teik-Cheng Lim. Mathematical relationships between bond-bending force fields. *Journal of Mathematical Chemistry*, 32(3):249–256, October 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022174923270`.

Vigo-Aguiar:2002:FTS

[832] J. Vigo-Aguiar and T. E. Simos. Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 32(3):257–270, October 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022127007340`.

Yildirim:2002:QSS

[833] Necmettin Yildirim. Quasi-steady state kinetics of simple sequential multienzyme reactions with single substrates. *Journal of Mathematical Chemistry*, 32(3):271–280, October 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022179124178`.

Campbell:2002:SSM

[834] J. D. Campbell, D. A. Harrington, P. van den Driessche, and J. Watmough. Stability of surface mechanisms with three species and mass–action kinetics. *Journal of Mathematical Chemistry*, 32(3):281–301, October 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022131208249`.

Marmorino:2002:ESH

[835] M. G. Marmorino. Exactly soluble Hamiltonian with a squared cotangent potential. *Journal of Mathematical Chemistry*, 32(3):303–308, October 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022183225087`.

Guseinov:2002:CMN

[836] I. I. Guseinov and B. A. Mamedov. Calculation of multicenter nuclear attraction and electron repulsion integrals over Slater orbitals by Fourier

transform method using Gegenbauer polynomials. *Journal of Mathematical Chemistry*, 32(4):309–322, November 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022926504733`.

Taseli:2002:EES

[837] H. Taseli, Inci M. Erhan, and Ö. Ugur. An eigenfunction expansion for the Schrödinger equation with arbitrary non-central potentials. *Journal of Mathematical Chemistry*, 32(4):323–338, November 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022949421571`.

Ezra:2002:GAR

[838] Gregory S. Ezra. Geometric approach to response theory in non–Hamiltonian systems. *Journal of Mathematical Chemistry*, 32(4):339–360, November 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022901505641`.

Leach:2002:CEV

[839] P. G. L. Leach, T. A. Ford, P. H. Matabal, and David P. White. Computation of the effective volumes of covalently bonded molecules. *Journal of Mathematical Chemistry*, 32(4):361–379, November 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022953522480`.

McKinney:2002:SESa

[840] Paul Caylor McKinney. Schrödinger equation solutions for the central field power potential energy I. $V(r) = V_0(r/a_0)^{2\nu-2}, \nu \geq 1$. *Journal of Mathematical Chemistry*, 32(4):381–404, November 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022905606550`.

McKinney:2002:SESb

[841] Paul Caylor McKinney. Schrödinger equation solutions for the central field power potential energy II. $V(r) = -V_0(r/a_0)^{2\nu-2}, 0 \leq \nu \leq 1$, the bound states. *Journal of Mathematical Chemistry*, 32(4):405–410, November 2002. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1022957623388`.

Aluffi-Pentini:2003:NAN

[842] F. Aluffi-Pentini, V. De Fonzo, and V. Parisi. A novel algorithm for the numerical integration of systems of ordinary differential equations

arising in chemical problems. *Journal of Mathematical Chemistry*, 33 (1):1–15, January 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1023295712640`.

Shiu:2003:ECR

[843] Wai Chee Shiu, Peter Che Bor Lam, and Lian zhu Zhang. Extremal k^*-cycle resonant hexagonal chains. *Journal of Mathematical Chemistry*, 33(1):17–28, January 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1023291329478`.

Lim:2003:MCB

[844] Teik-Cheng Lim. Mathematical connections between bond-stretching potential functions. *Journal of Mathematical Chemistry*, 33(1):29–37, January 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1023243413549`.

Zelentsov:2003:SPP

[845] Sergei V. Zelentsov, Samuel Kh. Aranson, and Leonid A. Belyakov. Solving the problem of photochemical kinetics in a medium with low reagent mobilities. *Journal of Mathematical Chemistry*, 33(1):39–54, January 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1023295430387`.

Miller:2003:SSM

[846] Gordon J. Miller and John G. Verkade. Shell structures in molecular orbital energy diagrams for "small" fullerene cages: Free-electron versus generator orbital models. *Journal of Mathematical Chemistry*, 33 (1):55–79, January 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1023247514457`.

Li:2003:OHW

[847] X. H. Li and J. J. Lin. The overall hyper–Wiener index. *Journal of Mathematical Chemistry*, 33(2):81–89, February 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1023299514399`.

Hollas:2003:AAD

[848] Boris Hollas. An analysis of the autocorrelation descriptor for molecules. *Journal of Mathematical Chemistry*, 33(2):91–101, February 2003. CO-

DEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1023247831238.

Doslic:2003:CEC

[849] Tomislav Doslić. Cyclical edge-connectivity of fullerene graphs and $(k, 6)$-cages. *Journal of Mathematical Chemistry*, 33(2):103–112, February 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1023299815308.

Fujita:2003:SAG

[850] Shinsaku Fujita. Stereogenicity/astereogenicity as global/local permutation-group symmetry and relevant concepts for restructuring stereochemistry. *Journal of Mathematical Chemistry*, 33(2):113–143, February 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1023251932146.

Avery:2003:GSM

[851] James Avery and John Avery. The generalized Sturmian method for calculating spectra of atoms and ions. *Journal of Mathematical Chemistry*, 33(2):145–162, February 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1023204016217.

March:2003:KED

[852] N. H. March and A. Holas. Kinetic energy density of the two-electron Hookean atom in terms of the ground-state electron density. *Journal of Mathematical Chemistry*, 33(2):163–170, February 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1023256000287.

Wang:2003:EIA

[853] Jianji Wang, Ruxiong Li, and Shen Wang. Enumeration of isomers of acyclic saturated hydroxyl ethers. *Journal of Mathematical Chemistry*, 33(3–4):171–179, May 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1024745122889.

Ozdogan:2003:CTC

[854] T. Özdogan, S. Gümüs, and M. Kara. Calculation of two-center nuclear attraction integrals over integer and noninteger n-Slater type orbitals in nonlined-up coordinate systems. *Journal of Mathematical Chemistry*, 33 (3–4):181–188, May 2003. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1024786506959. See comment [920].

Li:2003:CSC

[855] Xueliang Li, Haixing Zhao, and Lusheng Wang. A complete solution to a conjecture on the β-polynomials of graphs. *Journal of Mathematical Chemistry*, 33(3–4):189–193, May 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1024738623798.

Antippa:2003:LSP

[856] Adel F. Antippa. Lattice structure of phospholipidic molecular domains at the liquid–gas interface. *Journal of Mathematical Chemistry*, 33(3–4):195–225, May 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1024790607868.

Carbo-Dorca:2003:ASQ

[857] Ramon Carbó-Dorca. About some questions relative to the arbitrariness of signs: Their possible consequences in matrix signatures definition and quantum chemical applications. *Journal of Mathematical Chemistry*, 33 (3–4):227–244, May 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1024742724706.

Darowicki:2003:NMS

[858] Kazimierz Darowicki, Waldemar Felisiak, and Artur Zieliński. A novel method of spectral analysis of oscillatory Belousov–Zhabotinsky reaction. *Journal of Mathematical Chemistry*, 33(3–4):245–254, May 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1024794708776.

Fujita:2003:GMC

[859] Shinsaku Fujita and Sherif El-Basil. Graphical models of characters of groups. *Journal of Mathematical Chemistry*, 33(3–4):255–277, May 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1024746825615.

Lim:2003:SFB

[860] Teik-Cheng Lim. Scaling function between the exponential-6 and the generalized Lennard-Jones potential functions. *Journal of Mathematical Chemistry*, 33(3–4):279–285, May 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/A:1024798909685.

Benzal:2003:SNL

[861] G. Benzal, A. Kumar, A. M. Sastre, and A. Delshams. Simulation of nonlinear flow density in transition state from the mathematical model of the diffusion of metal anions through a flat sheet supported liquid membrane. *Journal of Mathematical Chemistry*, 34(1–2):1–27, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025133811600`.

Baeurle:2003:NFR

[862] Stephan Alexander Baeurle. On a new formulation of the real-time propagator. *Journal of Mathematical Chemistry*, 34(1–2):29–38, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025138528438`.

Simos:2003:FTF

[863] T. E. Simos. A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 34(1–2):39–58, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025190512508`.

Marmorino:2003:LBG

[864] M. G. Marmorino. Lower bounds to ground-state eigenvalues II. *Journal of Mathematical Chemistry*, 34(1–2):59–66, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025142604486`.

Bultinck:2003:NIF

[865] Patrick Bultinck and Ramon Carbó-Dorca. Negative and infinite Fukui functions: The role of diagonal dominance in the hardness matrix. *Journal of Mathematical Chemistry*, 34(1–2):67–74, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025136721324`.

Carbo-Dorca:2003:AGT

[866] Ramon Carbó-Dorca and Patrick Bultinck. Analysis of a general theorem concerning two non-commuting Hermitian matrices: Quantum mechanical implications for ground and excited states. *Journal of Mathematical Chemistry*, 34(1–2):75–82, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025188705395`.

Tselios:2003:SMN

[867] Kostas Tselios and T. E. Simos. Symplectic methods for the numerical solution of the radial Shrödinger equation. *Journal of Mathematical Chemistry*, 34(1–2):83–94, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025140822233`.

Yeh:2003:MPI

[868] Chin-Yah Yeh. A mathematical problem in isomerism and radicality of acyclic conjugated polyenes. *Journal of Mathematical Chemistry*, 34 (1–2):95–110, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025176529368`.

Zhang:2003:ECB

[869] Lian-Zhu Zhang and Feng Tian. Extremal catacondensed benzenoids. *Journal of Mathematical Chemistry*, 34(1–2):111–122, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025197913438`.

Ramasami:2003:CDO

[870] P. Ramasami. A concise description of an old problem: Application of matrices to obtain the balancing coefficients of chemical equations. *Journal of Mathematical Chemistry*, 34(1–2):123–129, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025150130276`.

Arrighini:2003:MAA

[871] G. P. Arrighini, S. Bruzzone, and C. Guidotti. More on the Airy averaging method. *Journal of Mathematical Chemistry*, 34(1–2):131–136, July 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/A:1025102214347`.

Iliev:2003:COC

[872] Valentin Vankov Iliev. On certain organic compounds with one monosubstitution and at least three di-substitution homogeneous derivatives. *Journal of Mathematical Chemistry*, 34(3–4):137–150, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004064.40608.c4`.

Lim:2003:SCA

[873] Teik-Cheng Lim. Spring constant analogy for estimating stiffness of a single polyethylene molecule. *Journal of Mathematical Chemistry*, 34(3–4):151–161, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004065.34221.47`.

Kaly-Kullai:2003:FMS

[874] Kristóf Kály-Kullai. A fast method to simulate travelling waves in nonhomogeneous chemical or biological media. *Journal of Mathematical Chemistry*, 34(3–4):163–176, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004066.71858.06`.

Taseli:2003:SHW

[875] H. Taseli and M. Bahar Erseçen. The scaled Hermite–Weber basis still highly competitive. *Journal of Mathematical Chemistry*, 34(3–4):177–187, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004067.16089.02`.

Schmalz:2003:BLD

[876] T. G. Schmalz, M. T. Pena, and E. T. Morgenthaler. Bond length dependence of cluster expansions of pi-electron energy. *Journal of Mathematical Chemistry*, 34(3–4):189–199, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004068.75704.e1`.

Sinha:2003:TDC

[877] Anjana Sinha. Three-dimensional confinement: WKB revisited. *Journal of Mathematical Chemistry*, 34(3–4):201–213, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004069.61693.c1`.

Lim:2003:EPP

[878] Teik-Cheng Lim. Elastic properties of a polyethylene single-molecule. *Journal of Mathematical Chemistry*, 34(3–4):215–220, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004070.49165.fe`.

Lim:2003:ENL

[879] Teik-Cheng Lim. Exact non-linear relationship between exponential-6 and Lennard-Jones (12–6) potential functions. *Journal of Mathematical Chemistry*, 34(3–4):221–225, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004071.86802.e9`.

Baronas:2003:MAB

[880] R. Baronas, F. Ivanauskas, J. Kulys, and M. Sapagovas. Modelling of amperometric biosensors with rough surface of the enzyme membrane. *Journal of Mathematical Chemistry*, 34(3–4):227–242, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004072.97338.12`.

Taseli:2003:EAS

[881] H. Taseli. Exact analytical solutions of the Hamiltonian with a squared tangent potential. *Journal of Mathematical Chemistry*, 34(3–4):243–251, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004073.17023.41`.

Arimoto:2003:NRS

[882] Shigeru Arimoto. Note on the repeat space theory. *Journal of Mathematical Chemistry*, 34(3–4):253–257, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004439.58582.e1`.

Arimoto:2003:NPF

[883] Shigeru Arimoto. New proof of the Fukui conjecture by the functional asymptotic linearity theorem. *Journal of Mathematical Chemistry*, 34(3–4):259–285, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004074.77942.9a`.

Arimoto:2003:FDE

[884] Shigeru Arimoto. The functional delta existence theorem and the reduction of a proof of the Fukui conjecture to that of the special functional asymptotic linearity theorem. *Journal of Mathematical Chemistry*, 34(3–4):287–296, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004075.59536.b9`.

Karimi:2003:DBF

[885] Sasan Karimi, Marty Lewinter, and Julian Stauffer. Double bonds in fused hexacyclic systems. *Journal of Mathematical Chemistry*, 34(3–4): 297–301, November 2003. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000004440.36576.9d`.

Arteca:2004:CBG

[886] Gustavo A. Arteca and O. Tapia. Comparison between a generalized electronic diabatic approach and the Born–Oppenheimer separation scheme in inertial frames. *Journal of Mathematical Chemistry*, 35(1):1–19, January 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000007809.83562.52`.

Lo:2004:CFR

[887] Shun S. Lo and Daniel A. Morales. A closed-form relation for dimension-dependent two-electron matrix elements of the interelectronic distance. *Journal of Mathematical Chemistry*, 35(1):21–28, January 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000007810.35417.20`.

Ezra:2004:SMN

[888] Gregory S. Ezra. On the statistical mechanics of non–Hamiltonian systems: The generalized Liouville equation, entropy, and time–dependent metrics. *Journal of Mathematical Chemistry*, 35(1):29–53, January 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000007811.79716.4d`.

Tselios:2004:SMF

[889] Kostas Tselios and T. E. Simos. Symplectic methods of fifth order for the numerical solution of the radial Shrödinger equation. *Journal of Mathematical Chemistry*, 35(1):55–63, January 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000007812.39332.fa`.

Alis:2004:IQM

[890] Ömer F. Alis, Herschel Rabitz, M. Q. Phan, C. Rosenthal, and M. Pence. On the inversion of quantum mechanical systems: Determining the amount and type of data for a unique solution. *Journal of Mathematical*

Chemistry, 35(1):65–78, January 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000007813.70019.39`.

Marmorino:2004:UBE

[891] M. G. Marmorino. Upper bound to the expectation value of the squared Hamiltonian. *Journal of Mathematical Chemistry*, 35(1):79–85, January 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000007814.41723.6b`.

Zhang:2004:ROE

[892] Fuji Zhang and Lusheng Wang. k-resonance of open-ended carbon nanotubes. *Journal of Mathematical Chemistry*, 35(2):87–103, February 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000014306.86197.22`.

Torres:2004:BRA

[893] Emilio Martínez Torres. Burnside rings: Application to molecules of icosahedral symmetry. *Journal of Mathematical Chemistry*, 35(2):105–117, February 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000014307.75757.13`.

Nelson:2004:FLO

[894] M. I. Nelson and H. S. Sidhu. Flammability limits of an oxidation reaction in a batch reactor. II. The Rychlý mechanism. *Journal of Mathematical Chemistry*, 35(2):119–129, February 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000014308.66514.e7`.

Ferreira:2004:TAC

[895] Chelo Ferreira, José L. López, and Pedro Miana. Two algorithms for computing the Randles–Sevcik function from electrochemistry. *Journal of Mathematical Chemistry*, 35(2):131–137, February 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000014309.04152.87`.

Bodroza-Pantic:2004:GFA

[896] Olga Bodroza-Pantić and Rade Doroslovacki. The Gutman formulas for algebraic structure count. *Journal of Mathematical Chemistry*, 35(2):139–146, February 2004. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000014310.56075.45.

Petitjean:2004:SSS

[897] Michel Petitjean. From shape similarity to shape complementarity: Toward a docking theory. *Journal of Mathematical Chemistry*, 35(3):147–158, March 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000033252.59423.6b.

Arteca:2004:TSM

[898] Gustavo A. Arteca and O. Tapia. A three-state model for electronic transitions represented in a generalized diabatic approach. *Journal of Mathematical Chemistry*, 35(3):159–174, March 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000033253.41017.0c.

Yan:2004:PPS

[899] Weigen Yan and Fuji Zhang. On the permanental polynomials of some graphs. *Journal of Mathematical Chemistry*, 35(3):175–188, March 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000033254.54822.f8.

Marmorino:2004:STL

[900] M. G. Marmorino and Pritha Gupta. Surpassing the Temple lower bound. *Journal of Mathematical Chemistry*, 35(3):189–197, March 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000033255.72679.f7.

Baronas:2004:EDL

[901] R. Baronas, F. Ivanauskas, and J. Kulys. The effect of diffusion limitations on the response of amperometric biosensors with substrate cyclic conversion. *Journal of Mathematical Chemistry*, 35(3):199–213, March 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000033256.70413.f7.

Paldus:2004:GMS

[902] Josef Paldus, Xiangzhu Li, and Nicholas D. K. Petraco. General-model-space state-universal coupled-cluster method: Diagrammatic approach. *Journal of Mathematical Chemistry*, 35(3):215–251, March

2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000033257.87377.1f.

Hinch:2004:MEE

[903] R. Hinch and S. Schnell. Mechanism equivalence in enzyme-substrate reactions: Distributed differential delay in enzyme kinetics. *Journal of Mathematical Chemistry*, 35(3):253–264, March 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000033258.42803.60.

Fujita:2004:IDS

[904] Shinsaku Fujita. Integrated discussion on stereogenicity and chirality for restructuring stereochemistry. *Journal of Mathematical Chemistry*, 35(3):265–287, March 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000033259.61553.25.

Site:2004:NIC

[905] L. Delle Site. A note on the initial condition of the differential equation which defines proper quantum topological subspaces. *Journal of Mathematical Chemistry*, 35(3):289–295, March 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000033260.32364.bb.

Wang:2004:ADL

[906] Xiaoyan Wang and Shiliang Ding. An application of the dynamical Lie algebraic method to potential energy surface of the stable linear asymmetric tetratomic molecules. *Journal of Mathematical Chemistry*, 35(4):297–307, April 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000034248.67399.1d.

Simon:2004:SSC

[907] Peter L. Simon, Stephen K. Scott, Serafim Kalliadasis, and John H. Merkin. On the structure of the spectra for a class of combustion waves. *Journal of Mathematical Chemistry*, 35(4):309–328, April 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000034249.20215.1f.

Teleki:2004:EOP

[908] Aba Teleki and Teodor Obert. Evaluation of the 3rd order perturbations for the degenerate cases. *Journal of Mathematical Chemistry*, 35 (4):329–338, April 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000034250.41575.ee`.

Bocchi:2004:DBC

[909] Timothy Bocchi, Marty Lewinter, and Sasan Karimi. On the distribution of π bonds in cyclofusene. *Journal of Mathematical Chemistry*, 35 (4):339–344, April 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000034251.23168.fb`.

Balasubramanian:2004:MCG

[910] K. Balasubramanian. Multinomial combinatorial group representations of the octahedral and cubic symmetries. *Journal of Mathematical Chemistry*, 35(4):345–365, April 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000034252.38828.a3`.

Taseli:2004:COP

[911] H. Taseli. A class of orthogonal polynomials suggested by a trigonometric Hamiltonian: Symmetric states. *Journal of Mathematical Chemistry*, 36(1):1–12, May 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000034929.23960.4e`.

Simos:2004:EFM

[912] T. E. Simos. Exponentially-fitted multiderivative methods for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 36(1):13–27, May 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000034930.81720.47`.

Turulski:2004:EBI

[913] Jan Turulski and Jan Niedzielski. Earth's biodiversity as interpreted by a chemist. *Journal of Mathematical Chemistry*, 36(1):29–40, May 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000034931.23685.df`.

Carbo-Dorca:2004:HRD

[914] Ramon Carbó-Dorca. Heisenberg's relations in discrete N-dimensional parameterized metric vector spaces. *Journal of Mathematical Chemistry*, 36(1):41–54, May 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000034932.49577.9a`.

Aragon:2004:ASP

[915] Sergio Aragon. The algebraic structure of physical quantities. *Journal of Mathematical Chemistry*, 36(1):55–74, May 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000034933.47311.93`.

Carbo-Dorca:2004:IDT

[916] Ramon Carbó-Dorca. Infinite-dimensional time vectors as background building blocks of a space–time frame structure. *Journal of Mathematical Chemistry*, 36(1):75–81, May 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000034934.13520.4f`.

Guseinov:2004:AEM

[917] I. I. Guseinov. Analytical evaluation of multicenter multielectron integrals of central and noncentral interaction potentials over Slater orbitals using overlap integrals and auxiliary functions. *Journal of Mathematical Chemistry*, 36(2):83–91, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000038774.73562.19`.

Amovilli:2004:EES

[918] Claudio Amovilli, Frederik E. Leys, and Norman H. March. Electronic energy spectrum of two-dimensional solids and a chain of C atoms from a quantum network model. *Journal of Mathematical Chemistry*, 36(2):93–112, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000038775.67243.f2`.

Guseinov:2004:EME

[919] I. I. Guseinov and B. A. Mamedov. Evaluation of multicenter electronic attraction, electric field and electric field gradient integrals with screened and nonscreened Coulomb potentials over integer and noninteger n Slater orbitals. *Journal of Mathematical Chemistry*, 36(2):113–121,

June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000038777.35582.d0.

Guseinov:2004:CCT

[920] I. I. Guseinov. Comment on "Calculation of Two-Center Nuclear Attraction Integrals over Integer and Noninteger n-Slater-Type Orbitals in Nonlined-Up Coordinate Systems". *Journal of Mathematical Chemistry*, 36(2):123–127, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000038771.04263.ec. See [854] and reply [1027].

Xian:2004:NPA

[921] Bi Xian, Tonghua Li, Chen Kai, Tongcheng Cao, Jianrong Huang, and Yunpeng Qi. A novel preprocessing algorithm for three-way HPLC data. *Journal of Mathematical Chemistry*, 36(2):129–138, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000038776.13329.72.

Lim:2004:RBM

[922] Teik-Cheng Lim. Relationship between Morse and Murrell–Mottram potentials at long range. *Journal of Mathematical Chemistry*, 36(2):139–145, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000038773.33727.e3.

Lim:2004:AMS

[923] Teik-Cheng Lim. Application of Maclaurin series in relating interatomic potential functions: A review. *Journal of Mathematical Chemistry*, 36 (2):147–160, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000038772.74111.05.

Fernandez:2004:RAP

[924] Francisco M. Fernández and Eduardo A. Castro. Relationships among potential-energy functions. *Journal of Mathematical Chemistry*, 36(2): 161–165, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000038790.56557.63.

Balasubramanian:2004:NT

[925] K. Balasubramanian. Number theory. *Journal of Mathematical Chemistry*, 36(2):167, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1023/B:JOMC.0000038791.72217.20.

Kazantzis:2004:NDS

[926] Nikolaos Kazantzis and Raymond A. Wright. On the nonlinear dynamic state reconstruction problem for chemical/biochemical reaction systems in the presence of model uncertainty. *Journal of Mathematical Chemistry*, 36(2):169–190, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000038792.47836.ad.

Bultinck:2004:MDD

[927] Patrick Bultinck and Ramon Carbó-Dorca. A mathematical discussion on density and shape functions, vector semispaces and related questions. *Journal of Mathematical Chemistry*, 36(2):191–200, June 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000038793.21806.65.

Carbo-Dorca:2004:GPO

[928] Ramon Carbó-Dorca and Patrick Bultinck. A general procedure to obtain quantum mechanical charge and bond order molecular parameters. *Journal of Mathematical Chemistry*, 36(3):201–210, July 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000044219.02356.be.

Fujita:2004:DCG

[929] Shinsaku Fujita and Sherif El-Basil. Doubly-colored graphs as graphical models for subductions of coset representations, double cosets, and unit subduced cycle indices. *Journal of Mathematical Chemistry*, 36 (3):211–229, July 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000044220.42054.1b.

Carbo-Dorca:2004:QMB

[930] Ramon Carbó-Dorca and Patrick Bultinck. Quantum mechanical basis for Mulliken population analysis. *Journal of Mathematical Chemistry*, 36(3):231–239, July 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000044221.23647.20.

Carbo-Dorca:2004:NLT

[931] Ramon Carbó-Dorca. Non-linear terms & variational approach in quantum QSPR. *Journal of Mathematical Chemistry*, 36(3):241–260, July 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044222.02974.ef`.

Lim:2004:CAC

[932] Teik-Cheng Lim. Connection among classical interatomic potential functions. *Journal of Mathematical Chemistry*, 36(3):261–269, July 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044223.40611.00`.

Vukicevic:2004:PER

[933] Damir Vukicević, Milan Randić, and Alexandru T. Balaban. Partitioning of π-electrons in rings of polycyclic conjugated hydrocarbons. Part 4. Benzenoids with more than one geometric Kekulé structure corresponding to the same algebraic Kekulé structure. *Journal of Mathematical Chemistry*, 36(3):271–279, July 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044224.17436.8a`.

Baronas:2004:AMU

[934] R. Baronas, F. Ivanauskas, R. Maslovskis, and P. Vaitkus. An analysis of mixtures using amperometric biosensors and artificial neural networks. *Journal of Mathematical Chemistry*, 36(3):281–297, July 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044225.76158.8e`.

Temme:2004:E

[935] F. P. Temme. Erratum. *Journal of Mathematical Chemistry*, 36(3):299–300, July 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1023/B:JOMC.0000044459.50613.e3`.

Mamedov:2004:EBF

[936] B. A. Mamedov. On the evaluation of Boys functions using downward recursion relation. *Journal of Mathematical Chemistry*, 36(3):301–306, July 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044226.49921.f5`.

Hirsch:2004:RPC

[937] Michael Hirsch and Wolfgang Quapp. Reaction pathways and convexity of the potential energy surface: Application of Newton trajectories. *Journal of Mathematical Chemistry*, 36(4):307–340, August 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044520.03226.5f`.

Guseinov:2004:EIG

[938] I. I. Guseinov and B. A. Mamedov. Evaluation of incomplete gamma functions using downward recursion and analytical relations. *Journal of Mathematical Chemistry*, 36(4):341–346, August 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044521.18885.d3`. See correction [3678].

Fossas:2004:PBC

[939] Enric Fossas, Rosa M. Ros, and Herbet Sira-Ramírez. Passivity-based control of a bioreactor system. *Journal of Mathematical Chemistry*, 36 (4):347–360, August 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044522.36742.4b`.

Besalu:2004:EPP

[940] E. Besalú and J. V. de Julián-Ortiz. Equivalence of the Pecka–Ponec correlation probability and the statistical F significance for MLR models. *Journal of Mathematical Chemistry*, 36(4):361–363, August 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044523.96357.49`.

Quapp:2004:NTC

[941] Wolfgang Quapp. Newton trajectories in the curvilinear metric of internal coordinates. *Journal of Mathematical Chemistry*, 36(4):365–379, August 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1023/B:JOMC.0000044524.48281.2d`.

Bucknum:2004:SDF

[942] Michael J. Bucknum and Eduardo A. Castro. Spiroconjugation in 1-, 2-, and 3-dimensions: The foundations of a spiro quantum chemistry. *Journal of Mathematical Chemistry*, 36(4):381–408, August

2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000044525.92511.ab.

Baeurle:2004:MEI

[943] Stephan A. Baeurle and Juergen Kroener. Modeling effective interactions of micellar aggregates of ionic surfactants with the Gauss-core potential. *Journal of Mathematical Chemistry*, 36(4):409–421, August 2004. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1023/B:JOMC.0000044526.22457.bb.

Lai:2005:PPA

[944] Shan-Tao Lai, Ying-Nan Chiu, and Ricardo Letelier. The primitive L-pattern of angular momentum recoupling coefficients. *Journal of Mathematical Chemistry*, 37(1):1–16, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-004-7659-z.

Min:2005:AEI

[945] Zhang Shi Min. Approximate expression for interaction of a two similar plane double layer at moderate and low potential. *Journal of Mathematical Chemistry*, 37(1):17–26, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-004-7660-6.

Ozdogan:2005:ETC

[946] Telhat Özdogan, Metin Orbay, and Salih Degirmenci. Evaluation of two-center overlap integrals using Slater type orbitals in terms of Bessel type orbitals. *Journal of Mathematical Chemistry*, 37(1):27–36, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-004-7661-5.

Hu:2005:SFH

[947] Qian-Nan Hu, Yi-Zeng Liang, Qing-Song Xu, Kai-Tai Fang, Xiao-Ling Peng, and Hong Yin. Structural features hidden in the degree distributions of topological graphs. *Journal of Mathematical Chemistry*, 37 (1):37–56, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-004-7662-4.

Kalachev:2005:GBA

[948] L. V. Kalachev and K. R. Schneider. Global behavior and asymptotic reduction of a chemical kinetics system with continua of equilibria. *Jour-*

nal of Mathematical Chemistry, 37(1):57–74, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-7663-3`.

Arimoto:2005:PFCa

[949] Shigeru Arimoto, Mark Spivakovsky, Keith F. Taylor, and Paul G. Mezey. Proof of the Fukui conjecture via resolution of singularities and related methods. I. *Journal of Mathematical Chemistry*, 37(1):75–91, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-7664-2`.

Qiao:2005:AAR

[950] Yu Qiao, Xinguo Kong, and Srinivas S. Chakravarthula. An analysis of aggregate response of confined liquids in nanoenvironment. *Journal of Mathematical Chemistry*, 37(2):93–99, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1442-z`.

Berberan-Santos:2005:CQS

[951] Mário N. Berberan-Santos, Evgeny N. Bodunov, and Lionello Pogliani. Classical and quantum study of the motion of a particle in a gravitational field. *Journal of Mathematical Chemistry*, 37(2):101–115, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1443-y`.

Cash:2005:CFH

[952] Gordon G. Cash. Coulson function and Hosoya index: extension of the relationship to polycyclic graphs and to new types of matching polynomials. *Journal of Mathematical Chemistry*, 37(2):117–125, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1444-x`.

He:2005:CQT

[953] Jianfeng He, Wei Hua, Xueshen Liu, and Peizhu Ding. Computation of quasiclassical trajectories by symplectic algorithm for the $N(^4S) + O_2 (X^3\Sigma_g)^- \rightarrow NO(X^2\Pi) + O(^3P)$ reaction system. *Journal of Mathematical Chemistry*, 37(2):127–138, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1445-9`.

Aktas:2005:ESS

[954] Metin Aktas and Ramazan Sever. Exact solution of Schrödinger equation with deformed ring-shaped potential. *Journal of Mathematical Chem-*

istry, 37(2):139–148, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1446-8`.

Gubernov:2005:EAT

[955] V. V. Gubernov, H. S. Sidhu, and G. N. Mercer. The effect of ambient temperature on the propagation of nonadiabatic combustion waves. *Journal of Mathematical Chemistry*, 37(2):149–162, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1447-7`.

Vukicevic:2005:CDP

[956] D. Vukicević and D. J. Klein. Characterization of distribution of pi-electrons amongst benzenoid rings for Randić's "algebraic" Kekulé structures. *Journal of Mathematical Chemistry*, 37(2):163–170, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1448-6`.

Arimoto:2005:PFCb

[957] Shigeru Arimoto, Mark Spivakovsky, Keith F. Taylor, and Paul G. Mezey. Proof of the Fukui conjecture via resolution of singularities and related methods. II*. *Journal of Mathematical Chemistry*, 37(2):171–189, January 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1449-5`.

Nikolopoulos:2005:NBA

[958] L. A. A. Nikolopoulos. A numerical basis for the accurate representation of the continuum spectrum of atomic Hamiltonians. *Journal of Mathematical Chemistry*, 37(3):191–199, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1462-8`.

Simos:2005:PSI

[959] T. E. Simos. Preface for the special issue on the International Conference of Computational Methods in Sciences and Engineering 2003 (ICCMSE 2003). *Journal of Mathematical Chemistry*, 37(3):201, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-004-1463-7`; `http://link.springer.com/article/10.1007/s10910-004-1463-7`.

Nikolopoulos:2005:FEA

[960] L. A. A. Nikolopoulos. A finite element approach for the continuum spectrum of the Dirac radial equation. *Journal of Mathematical Chemistry*, 37(3):203–210, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1464-6`.

Valderrama:2005:ECS

[961] Elmer G. Valderrama and Jesus M. Ugalde. Electron correlation studies by means of local-scaling transformations and electron-pair density functions. *Journal of Mathematical Chemistry*, 37(3):211–231, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1465-5`.

Emiris:2005:MCS

[962] Ioannis Z. Emiris and Theodoros G. Nikitopoulos. Molecular conformation search by distance matrix perturbations. *Journal of Mathematical Chemistry*, 37(3):233–253, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1466-4`.

Vigo-Aguiar:2005:VSN

[963] Jesús Vigo-Aguiar and Higinio Ramos. A variable-step Numerov method for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 37(3):255–262, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1467-3`.

Monovasilis:2005:EFS

[964] Th. Monovasilis, Z. Kalogiratou, and T. E. Simos. Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 37(3):263–270, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1468-2`.

Kalogiratou:2005:NST

[965] Z. Kalogiratou, Th. Monovasilis, and T. E. Simos. Numerical solution of the two-dimensional time independent Schrödinger equation with Numerov-type methods. *Journal of Mathematical Chemistry*, 37 (3):271–279, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1469-1`.

Anastassi:2005:TFR

[966] Z. A. Anastassi and T. E. Simos. Trigonometrically fitted Runge–Kutta methods for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 37(3):281–293, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1470-8`.

Psihoyios:2005:SAO

[967] G. Psihoyios and T. E. Simos. Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation. *Journal of Mathematical Chemistry*, 37(3): 295–316, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1471-7`.

Sakas:2005:FMM

[968] D. P. Sakas and T. E. Simos. A family of multiderivative methods for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 37(3):317–332, April 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1472-6`.

Hao:2005:ADG

[969] Jianxiu Hao. The adjoints of DNA graphs. *Journal of Mathematical Chemistry*, 37(4):333–346, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1099-7`.

Rodrigues:2005:ICE

[970] Alexandre Carlos Camacho Rodrigues. Influence of the composition on the electronegativity and on the oxygen charge distribution in a binary hydrotalcite-like by modified Sanderson method. *Journal of Mathematical Chemistry*, 37(4):347–351, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1100-5`.

Guseinov:2005:CME

[971] I. I. Guseinov and B. A. Mamedov. Calculation of multicenter electronic attraction, electric field and electric field gradient integrals of Coulomb potential over integer and noninteger n Slater orbitals. *Journal of Mathematical Chemistry*, 37(4):353–364, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1102-3`.

Ivanauskas:2005:MSS

[972] Feliksas Ivanauskas, Aivaras Kareiva, and Bogdanas Lapcun. On the modelling of solid state reactions.synthesis of YAG. *Journal of Mathematical Chemistry*, 37(4):365–376, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1103-2`.

Taseli:2005:COP

[973] H. Taseli. A class of orthogonal polynomials suggested by a trigonometric Hamiltonian: Antisymmetric states. *Journal of Mathematical Chemistry*, 37(4):377–388, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1104-1`.

Arteca:2005:QTC

[974] Gustavo A. Arteca and O. Tapia. A quantum theory of chemical processes and reaction rates based on diabatic electronic functions coupled in an external field. *Journal of Mathematical Chemistry*, 37(4):389–408, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1105-0`.

Bandstra:2005:CLT

[975] Joel Z. Bandstra and Paul G. Tratnyek. Central limit theorem for chemical kinetics in complex systems. *Journal of Mathematical Chemistry*, 37(4):409–422, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1107-y`.

Zhang:2005:BGM

[976] Jianbin Zhang and Bo Zhou. On bicyclic graphs with minimal energies. *Journal of Mathematical Chemistry*, 37(4):423–431, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1108-x`.

Castro:2005:QME

[977] Eduardo A. Castro, Francisco M. Fernández, and Pablo R. Duchowicz. QSPR modeling of the enthalpy of formation based on partial order ranking. *Journal of Mathematical Chemistry*, 37(4):433–441, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1110-3`.

Balaban:2005:PER

[978] Alexandru T. Balaban and Milan Randić. Partitioning of π-electrons in rings of polycyclic conjugated hydrocarbons: Part 6. Comparison with other methods for estimating the local aromaticity of rings in polycyclic benzenoids. *Journal of Mathematical Chemistry*, 37(4):443–453, May 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-1114-z`.

Maggiora:2005:ITC

[979] Gerald M. Maggiora and Veerabahu Shanmugasundaram. An information-theoretic characterization of partitioned property spaces. *Journal of Mathematical Chemistry*, 38(1):1–20, July 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-4525-6`.

Guseinov:2005:FEM

[980] I. I. Guseinov and B. A. Mamedov. Fast evaluation of molecular auxiliary functions A_α and B_n by analytical relations. *Journal of Mathematical Chemistry*, 38(1):21–26, July 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-4527-4`.

Bucknum:2005:TMT

[981] Michael J. Bucknum and Eduardo A. Castro. Towards a microscopic theory of the modulus of elasticity in crystalline covalent materials and a survey of potential superhard materials. *Journal of Mathematical Chemistry*, 38(1):27–42, July 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-4528-3`.

Nalewajski:2005:EIB

[982] Roman F. Nalewajski. Entropy/information bond indices of molecular fragments. *Journal of Mathematical Chemistry*, 38(1):43–66, July 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-4529-2`.

Varon:2005:TBM

[983] R. Varón, M. García-Moreno, M. Ll. Amo, E. Valero, F. García-Sevilla, and F. García-Molina. Time behaviour of the modifier involved in the general mechanism of botts and Morales assuming rapid equilibrium in the modifier bindings. *Journal of Mathematical Chemistry*, 38(1):67–88,

July 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-4530-9.

Carbo-Dorca:2005:DHR

[984] Ramon Carbó-Dorca. Deduction of Heisenberg relations and Schrödinger equation through the structure of N-dimensional parameterized metric vector spaces. *Journal of Mathematical Chemistry*, 38(1):89–101, July 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-4531-8.

Karimi:2005:ISB

[985] Sasan Karimi and Marty Lewinter. Interpolation of shared π-bonds in cyclofusene. *Journal of Mathematical Chemistry*, 38(1):103–106, July 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-4534-5.

Huang:2005:CSC

[986] Yan Huang and Xiao-Song Yang. Chaoticity of some chemical attractors: a computer assisted proof. *Journal of Mathematical Chemistry*, 38(1):107–117, July 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-4537-2.

Zhu:2005:RPL

[987] Lemin Zhu and Xuncheng Huang. Relative positions of limit cycles in the continuous culture vessel with variable yield. *Journal of Mathematical Chemistry*, 38(2):119–128, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-4837-6.

Shimin:2005:GRE

[988] Zhang Shimin. The graphical representation of equilibrium for the isothermal and isobaric reactions of ideal gases. *Journal of Mathematical Chemistry*, 38(2):129–140, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-4838-5.

Shimin:2005:SCP

[989] Zhang Shimin. The stability condition of phase equilibrium for various concentration variables. *Journal of Mathematical Chemistry*, 38(2):141–163, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-4839-4.

Berberan-Santos:2005:AIL

[990] Mário N. Berberan-Santos. Analytical inversion of the Laplace transform without contour integration: application to luminescence decay laws and other relaxation functions. *Journal of Mathematical Chemistry*, 38(2): 165–173, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-4961-3.

Fujita:2005:CEE

[991] Shinsaku Fujita. Combinatorial enumeration of ethane derivatives as three-dimensional chemical structures, not as graphs. A systematic approach for enumerating and characterizing stereoisomers of tartaric acids and related compounds. *Journal of Mathematical Chemistry*, 38(2): 175–194, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-5189-y.

Lim:2005:CAP

[992] Teik-Cheng Lim. Correlation among parameters of the extended-Rydberg potential energy function. *Journal of Mathematical Chemistry*, 38(2):195–201, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-5282-2.

Simon:2005:ERS

[993] Peter L. Simon, Stephen K. Scott, Serafim Kalliadasis, and John H. Merkin. The effect of a radical scavenger on the propagation of flames in an exothermic-endothermic system. *Journal of Mathematical Chemistry*, 38(2):203–231, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-5409-5.

Qian:2005:NKS

[994] Jianguo Qian and Fuji Zhang. On the number of Kekulé structures in capped zigzag nanotubes. *Journal of Mathematical Chemistry*, 38 (2):233–246, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-5410-z.

Daza:2005:EBI

[995] Edgar Eduardo Daza and Andrés Bernal. Energy bounds for isoelectronic molecular sets and the implicated order. *Journal of Mathematical Chemistry*, 38(2):247–263, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5411-y`.

Berberan-Santos:2005:RBI

[996] Mário N. Berberan-Santos. Relation between the inverse Laplace transforms of $I(t^\beta)$ and $I(t)$: Application to the Mittag-Leffler and asymptotic inverse power law relaxation functions. *Journal of Mathematical Chemistry*, 38(2):265–270, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5412-x`.

Abad:2005:FAD

[997] A. Abad, S. C. Cardona, J. I. Torregrosa, F. López, and J. Navarro-Laboulais. Flow analysis deconvolution for kinetic information reconstruction. *Journal of Mathematical Chemistry*, 38(2):271–292, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5422-8`.

Wang:2005:OBC

[998] Lusheng Wang, Fuji Zhang, and Hao Zhao. On the ordering of benzenoid chains and cyclo-polyphenacenes with respect to their numbers of Clar aromatic sextets. *Journal of Mathematical Chemistry*, 38(2): 293–309, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5423-7`.

Guseinov:2005:UAR

[999] I. I. Guseinov and B. A. Mamedov. Use of analytical relations in evaluation of exponential integral functions. *Journal of Mathematical Chemistry*, 38(2):311–314, August 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5426-4`.

Zhang:2005:CBF

[1000] Heping Zhang and Jinghua He. A comparison between 1-factor count and resonant pattern count in plane non-bipartite graphs. *Journal of*

Mathematical Chemistry, 38(3):315–324, October 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5821-x`.

Kotdawala:2005:AMF

[1001] Rasesh R. Kotdawala, Nikolaos Kazantzis, and Robert W. Thompson. An application of mean-field perturbation theory for the adsorption of polar molecules in nanoslit-pores. *Journal of Mathematical Chemistry*, 38 (3):325–344, October 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5823-8`.

Liu:2005:RI

[1002] Huiqing Liu, Mei Lu, and Feng Tian. On the Randić index. *Journal of Mathematical Chemistry*, 38(3):345–354, October 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5824-7`.

Ivanauskas:2005:CSS

[1003] F. Ivanauskas, I. Kaunietis, V. Laurinavicius, J. Razumiene, and R. Simkus. Computer simulation of the steady state currents at enzyme doped carbon paste electrodes. *Journal of Mathematical Chemistry*, 38 (3):355–366, October 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5825-6`.

Taseli:2005:SHW

[1004] H. Taseli and H. Alici. The scaled Hermite–Weber basis in the spectral and pseudospectral pictures. *Journal of Mathematical Chemistry*, 38 (3):367–378, October 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-5826-5`.

Hollas:2005:AIT

[1005] Boris Hollas. Asymptotically independent topological indices on random trees. *Journal of Mathematical Chemistry*, 38(3):379–387, October 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6474-5`.

Morales:2005:TEE

[1006] Daniel A. Morales. The total π-electron energy as a problem of moments: application of the Backus–Gilbert method. *Journal of Mathematical Chemistry*, 38(3):389–397, October 2005. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6475-4`.

Huang:2005:TDCa

[1007] Xuncheng Huang and Lemin Zhu. A three-dimensional chemostat with quadratic yields. *Journal of Mathematical Chemistry*, 38(3):399–412, October 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6476-3`.

Karimi:2005:E

[1008] Sasan Karimi and Marty Lewinter. Errata. *Journal of Mathematical Chemistry*, 38(3):413, October 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-005-8071-z; http://link.springer.com/article/10.1007/s10910-005-8071-z`.

Marmorino:2005:IWI

[1009] M. G. Marmorino. Improvement of Weyl's inequality. *Journal of Mathematical Chemistry*, 38(4):415–424, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-6893-8`. See comment [1131].

King:2005:CDK

[1010] R. Bruce King and Mircea V. Diudea. From the cube to the Dyck and Klein tessellations: Implications for the structures of zeolite-like carbon and boron nitride allotropes. *Journal of Mathematical Chemistry*, 38(4):425–435, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-6894-7`.

Varon:2005:TNR

[1011] R. Varón, M. García-Moreno, F. García-Molina, M. E. Fuentes, E. Arribas, J. M. Yago, M. Ll. Amo-Saus, and E. Valero. Two new regulatory properties arising from the transient phase kinetics of monocyclic enzyme cascades. *Journal of Mathematical Chemistry*, 38(4):437–450, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-004-6895-6`.

Shiu:2005:RTP

[1012] Wai Chee Shiu, Peter Che Bor Lam, and Heping Zhang. k-resonance in toroidal polyhexes*. *Journal of Mathematical Chemistry*, 38(4):451–

466, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-004-6897-4.

Huynh:2005:POD

[1013] Nguyen Huynh and Nikolaos Kazantzis. Parametric optimization of digitally controlled nonlinear reactor dynamics using Zubov-like functional equations. *Journal of Mathematical Chemistry*, 38(4):467–487, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-004-6899-2.

Guseinov:2005:ETT

[1014] I. I. Guseinov. Evaluation of two- and three-center overlap integrals over complete orthonormal sets of Ψ^{α}-ETOs using their addition theorems. *Journal of Mathematical Chemistry*, 38(4):489–493, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-004-6902-y.

Lim:2005:PFT

[1015] Teik-Cheng Lim. Polynomial forms of typical interatomic potential functions. *Journal of Mathematical Chemistry*, 38(4):495–501, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-004-6903-x.

Salem:2005:USC

[1016] Khaled Salem and Ivan Gutman. The unfixed subgraph of a catacondensed hexagonal system obtained by fixing an alternating set. *Journal of Mathematical Chemistry*, 38(4):503–510, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-004-6896-5.

Guseinov:2005:URA

[1017] I. I. Guseinov and B. A. Mamedov. Use of recursion and analytical relations in evaluation of hypergeometric functions arising in multicenter integrals with noninteger n Slater type orbitals. *Journal of Mathematical Chemistry*, 38(4):511–517, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-6904-4.

SegredeGiambiagi:2005:CEC

[1018] Myriam Segre de Giambiagi, Marçal Oliveira de Neto, and Amarílis V. Finageiv de Neder. Cooperative effect of CH$\cdots$O bonds in models

for biological systems. *Journal of Mathematical Chemistry*, 38(4):519–532, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6905-3`.

Faridfathi:2005:SSP

[1019] Gholamreza Faridfathi, Ramazan Sever, and Metin Aktas. Supersymmetric solutions of PT-/non-PT-symmetric and non–Hermitian central potentials via Hamiltonian hierarchy method. *Journal of Mathematical Chemistry*, 38(4):533–540, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6900-8`.

Abad:2005:TFF

[1020] A. Abad, S. C. Cardona, J. I. Torregrosa, F. López, and J. Navarro-Laboulais. On transfer function formalism for chemical reactor monitoring by continuous flow techniques. *Journal of Mathematical Chemistry*, 38(4):541–564, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6907-1`.

Fraga:2005:MSR

[1021] S. Fraga, J. M. García de la Vega, and E. S. Fraga. Molecular Schrödinger–Riccati calculations: The potential energy curve of the hydrogen molecule. *Journal of Mathematical Chemistry*, 38(4):565–573, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6906-2`.

Huang:2005:TDCb

[1022] Xuncheng Huang and Lemin Zhu. A three dimensional chemostat with quadratic yields. *Journal of Mathematical Chemistry*, 38(4):575–588, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6908-0`.

Heiberg-Andersen:2005:SCC

[1023] H. Heiberg-Andersen and A. T. Skjeltorp. Stability of conjugated carbon nanocones. *Journal of Mathematical Chemistry*, 38(4):589–604, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6913-3`.

Nelson:2005:ACM

[1024] M. I. Nelson and H. S. Sidhu. Analysis of a chemostat model with variable yield coefficient. *Journal of Mathematical Chemistry*, 38(4): 605–615, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6914-2`.

Doslic:2005:PMB

[1025] Tomislav Doslić. Perfect matchings in bipartite lattice animals: Lower bounds and realizability. *Journal of Mathematical Chemistry*, 38(4): 617–627, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6915-1`.

Berberan-Santos:2005:PML

[1026] Mário N. Berberan-Santos. Properties of the Mittag-Leffler relaxation function. *Journal of Mathematical Chemistry*, 38(4):629–635, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6909-z`.

Ozdogan:2005:RCC

[1027] Telhat Özdogan. Reply to "Comment on 'Calculation of Two-center Nuclear Attraction Integrals over Integer and Noninteger N-Slater-type Orbitals in Nonlined-up Coordinate Systems' ". *Journal of Mathematical Chemistry*, 38(4):637–640, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6912-4`. See [920].

Moharerrzadeh:2005:ATM

[1028] Mohammad Moharerrzadeh, Pancracio Palting, and Lue-Yung Chow Chiu. Addition theorem and matrix elements of radiative multipole operators. *Journal of Mathematical Chemistry*, 38(4):641–656, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6910-6`.

Merkin:2005:EEF

[1029] J. H. Merkin. The effect of an electric field on reaction fronts in autocatalytic systems. *Journal of Mathematical Chemistry*, 38(4):657–670, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6916-0`.

Carbo-Dorca:2005:MNF

[1030] Ramon Carbó-Dorca. Molecular nuclear fields: A Naïve perspective. *Journal of Mathematical Chemistry*, 38(4):671–676, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6911-5`.

Lu:2005:RIA

[1031] Mei Lu, Lian zhu Zhang, and Feng Tian. On the Randić index of acyclic conjugated molecules. *Journal of Mathematical Chemistry*, 38(4): 677–684, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6892-4`.

Jiang:2005:CSS

[1032] Wenyong Jiang, Zhengxia Chen, Yunhong Liu, Haifeng Zou, Junfeng Li, Hongyan Wang, and Wenyong Jiang. Computer simulation of surface tension for complex emulsion system. *Journal of Mathematical Chemistry*, 38(4):685–693, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6917-z`.

Mamedov:2005:EGE

[1033] B. A. Mamedov, Z. Merdan, and I. M. Askerov. Evaluation of generalized exponential integrals using multinomial expansion theorems. *Journal of Mathematical Chemistry*, 38(4):695–700, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6918-y`.

Darowicki:2005:ADW

[1034] Kazimierz Darowicki, Waldemar Felisiak, and Artur Zieliński. Application of discrete wavelet transform in the analysis of nonlinear chemical system. *Journal of Mathematical Chemistry*, 38(4):701–711, November 2005. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-6898-y`.

Gubernov:2006:CWM

[1035] V. V. Gubernov, H. S. Sidhu, and G. N. Mercer. Combustion waves in a model with chain branching reaction. *Journal of Mathematical Chemistry*, 39(1):1–14, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9000-x`.

Papp:2006:ESL

[1036] Dávid Papp and Béla Vizvári. Effective solution of linear Diophantine equation systems with an application in chemistry. *Journal of Mathematical Chemistry*, 39(1):15–31, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9001-9`.

Bucknum:2006:TFSa

[1037] Michael J. Bucknum and Eduardo A. Castro. On topological form in structures. *Journal of Mathematical Chemistry*, 39(1):33–46, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9002-8`.

Gluzman:2006:SSP

[1038] S. Gluzman and V. I. Yukalov. Self-similar power transforms in extrapolation problems. *Journal of Mathematical Chemistry*, 39(1):47–56, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9003-7`.

Moharerrzadeh:2006:ATM

[1039] Mohammad Moharerrzadeh, Pancracio Palting, and Lue-Yung Chow Chiu. Addition theorem and matrix elements of radiative multipole operators. *Journal of Mathematical Chemistry*, 39(1):57–72, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9005-5`.

Devadoss:2006:MIF

[1040] D. E. Devadoss and V. A. Volpert. Modeling isothermal free-radical frontal polymerization with gel effect using free volume theory, with and without inhibition. *Journal of Mathematical Chemistry*, 39(1): 73–105, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9006-4`.

Mestres:2006:PMS

[1041] Jordi Mestres and Gerald M. Maggiora. Putting molecular similarity into context: asymmetric indices for field-based similarity measures. *Journal of Mathematical Chemistry*, 39(1):107–118, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9007-3`.

Rajtmajer:2006:CAS

[1042] Sarah Michele Rajtmajer, Ante Milicević, Nenad Trinajstić, Milan Randić, and Damir Vukicević. On the complexity of Archimedean solids. *Journal of Mathematical Chemistry*, 39(1):119–132, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9008-2`.

Qi:2006:IDM

[1043] Yue-Ying Qi, Xue-Shen Liu, Xiao-Yan Liu, and Pei-Zhu Ding. Ionization of 1-D model atom in an intense laser field based on asymptotic boundary conditions and symplectic algorithm. *Journal of Mathematical Chemistry*, 39(1):133–149, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9009-1`.

Zivkovic:2006:IISa

[1044] Tomislav P. Zivković. Interaction of an isolated state with an infinite quantum system containing several one-parameter eigenvalue bands: II. time-dependent case. *Journal of Mathematical Chemistry*, 39(1): 151–176, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9010-8`.

Lim:2006:ABC

[1045] Teik-Cheng Lim. Application of binomial coefficients in representing central difference solution to a class of PDE arising in chemistry. *Journal of Mathematical Chemistry*, 39(1):177–186, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9011-7`.

Shimin:2006:GFP

[1046] Zhang Shimin. A generalized formula to predict the direction of an equilibrium shift. *Journal of Mathematical Chemistry*, 39(1):187–199, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9015-3`.

Jesudason:2006:EIP

[1047] Christopher G. Jesudason. An energy interconversion principle applied in reaction dynamics for the determination of equilibrium standard states. *Journal of Mathematical Chemistry*, 39(1):201–230, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9018-0`.

Wang:2006:UHM

[1048] Wen-Huan Wang, An Chang, Lian-Zhu Zhang, and Dong-Qiang Lu. Unicyclic Hückel molecular graphs with minimal energy. *Journal of Mathematical Chemistry*, 39(1):231–241, January 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9022-4`.

Cai:2006:MIC

[1049] Guang hui Cai. Moment inequalities and convergence rates in the strong laws for ρ^--mixing random fields. *Journal of Mathematical Chemistry*, 39 (2):243–251, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9028-y`.

Guseinov:2006:ORA

[1050] I. I. Guseinov. One-range addition theorems for combined Coulomb and Yukawa like central and noncentral interaction potentials and their derivatives. *Journal of Mathematical Chemistry*, 39(2):253–258, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9030-4`.

Gutman:2006:NCI

[1051] Ivan Gutman and Miodrag Mateljević. Note on the Coulson integral formula. *Journal of Mathematical Chemistry*, 39(2):259–266, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9032-2`.

Carbo-Dorca:2006:DEP

[1052] Ramon Carbó-Dorca. A discussion on the Einstein–Podolsky–Rosen (EPR) effect in a unique wavefunction quantum mechanical framework. *Journal of Mathematical Chemistry*, 39(2):267–279, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9031-3`.

Huang:2006:CBG

[1053] Xuncheng Huang, Yuanming Wang, and Lemin Zhu. Competition in the bioreactor with general quadratic yields when one competitor produces a toxin. *Journal of Mathematical Chemistry*, 39(2):281–294, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9040-2`.

Zivkovic:2006:IISb

[1054] Tomislav P. Zivković. Interaction of an isolated state with an infinite quantum system containing several one-parameter eigenvalue bands: I. Time-independent case. *Journal of Mathematical Chemistry*, 39(2): 295–344, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9014-4`.

Baronas:2006:CMB

[1055] R. Baronas, J. Kulys, and F. Ivanauskas. Computational modelling of biosensors with perforated and selective membranes. *Journal of Mathematical Chemistry*, 39(2):345–362, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9034-0`.

Restrepo:2006:TSCa

[1056] Guillermo Restrepo, Héber Mesa, and José L. Villaveces. On the topological sense of chemical sets. *Journal of Mathematical Chemistry*, 39(2): 363–376, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9013-5`.

Huang:2006:NAC

[1057] Yan Huang and Xiao-Song Yang. Numerical analysis on the complex dynamics in a chemical system. *Journal of Mathematical Chemistry*, 39 (2):377–387, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9043-z`.

Yan:2006:CBW

[1058] Weigen Yan and Yeong-Nan Yeh. Connections between Wiener index and matchings. *Journal of Mathematical Chemistry*, 39(2):389–399, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9026-0`.

Restrepo:2006:TSCb

[1059] Guillermo Restrepo, Eugenio J. Llanos, and Héber Mesa. Topological space of the chemical elements and its properties. *Journal of Mathematical Chemistry*, 39(2):401–416, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9041-1`.

Ruan:2006:TBR

[1060] Dong Ruan. Two-boson realizations of the polynomial angular momentum algebra and some applications. *Journal of Mathematical Chemistry*, 39(2):417–440, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9025-1`.

Shimin:2006:ISE

[1061] Zhang Shimin. Influence of substance on the equilibrium translation rate for the isothermal and isobaric chemical reactions of ideal gases. *Journal of Mathematical Chemistry*, 39(2):441–450, February 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9045-x`.

Zhang:2006:EEH

[1062] Chunli Zhang, Xueshen Liu, Peizhu Ding, and Yueying Qi. The enhancement of efficiency of high-order harmonic in intense laser field based on asymptotic boundary conditions and symplectic algorithm. *Journal of Mathematical Chemistry*, 39(3–4):451–463, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9042-0`.

Zhou:2006:MET

[1063] Bo Zhou and Feng Li. On minimal energies of trees of a prescribed diameter. *Journal of Mathematical Chemistry*, 39(3–4):465–473, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9047-8`.

Besalu:2006:OPP

[1064] Emili Besalú, J. Vicente de. Julián-Ortiz, Monica Iglesias, and Lionello Pogliani. An overlooked property of plot methods. *Journal of Mathematical Chemistry*, 39(3–4):475–484, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9035-z`.

LetelierD:2006:LCV

[1065] Jorge Ricardo Letelier D. and Alejandro Toro-Labbé. The linear combination of vibrational wave functions (LCVW) method in a Morse–Gaussian double well molecular potential. *Journal of Mathematical Chemistry*, 39(3–4):485–494, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9029-x`.

Carbo-Dorca:2006:GMF

[1066] Ramon Carbó-Dorca and Emili Besalú. Generation of molecular fields, quantum similarity measures and related questions. *Journal of Mathematical Chemistry*, 39(3–4):495–510, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9046-9`.

Kumar:2006:AGT

[1067] Vipin Kumar and A. K. Madan. Application of graph theory: Prediction of cytosolic phospholipase A_2 inhibitory activity of propan-2-ones. *Journal of Mathematical Chemistry*, 39(3–4):511–521, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9036-y`.

Michael:2006:SSL

[1068] George Michael. On a singular Sturm–Liouville problem in the theory of molecular vibrations. *Journal of Mathematical Chemistry*, 39 (3–4):523–539, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9037-x`.

Rodrigues:2006:EMS

[1069] Alexandre Carlos Camacho Rodrigues. Extension of the modified Sanderson method to ternary mixed oxides derived from hydrotalcite-like compounds and its correlation to CO_2 (TPD-CO_2) desorption peak maxima. *Journal of Mathematical Chemistry*, 39(3–4):541–549, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9033-1`.

Carbo-Dorca:2006:DPD

[1070] Ramon Carbó-Dorca. Descriptors and probability distributions in MO theory: Weighted Mulliken matrices and molecular quantum similarity measures. *Journal of Mathematical Chemistry*, 39(3–4):551–591, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9049-6`.

Karimi:2006:PCM

[1071] Sasan Karimi and Marty Lewinter. On the properties of convex multilayered cyclofusene. *Journal of Mathematical Chemistry*, 39(3–4):593–596, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9052-y`.

King:2006:CIF

[1072] R. Bruce. King and Mircea V. Diudea. The chirality of icosahedral fullerenes: a comparison of the tripling (leapfrog), quadrupling (chamfering), and septupling (Capra) transformations. *Journal of Mathematical Chemistry*, 39(3–4):597–604, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9048-7`.

Salem:2006:AIL

[1073] Khaled Salem and Hernán Abeledo. Alternative integer–linear-programming formulations of the Clar problem in hexagonal systems. *Journal of Mathematical Chemistry*, 39(3–4):605–610, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9051-z`.

Bucknum:2006:HHO

[1074] Michael J. Bucknum and Eduardo A. Castro. Hexagonite: A hypothetical organic zeolite. *Journal of Mathematical Chemistry*, 39(3–4):611–628, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9050-0`.

Luo:2006:RSS

[1075] Jiawei Luo, Bo Liao, Renfa Li, and Wen Zhu. RNA secondary structure 3D graphical representation without degeneracy. *Journal of Mathematical Chemistry*, 39(3–4):629–636, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9053-x`.

Tapia:2006:CCD

[1076] O. Tapia. Can chemistry be derived from quantum mechanics? Chemical dynamics and structure. *Journal of Mathematical Chemistry*, 39 (3–4):637–669, May 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9012-6`.

Vigo-Aguiar:2006:P

[1077] J. Vigo-Aguiar and B. A. Wade. Preface. *Journal of Mathematical Chemistry*, 40(1):1–2, July 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-006-9119-4; http://link.springer.com/article/10.1007/s10910-006-9119-4`.

Escobedo:2006:NMQ

[1078] Ramón Escobedo and Luis L. Bonilla. Numerical methods for a quantum drift-diffusion equation in semiconductor physics. *Journal of Mathematical Chemistry*, 40(1):3–13, July 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9122-9`.

Cuadrado:2006:MCS

[1079] Manuel Urbano Cuadrado, Gonzalo Cerruela García, Irene Luque Ruiz, and Miguel Ángel Gómez-Nieto. A method for clustering and screening of long-dimensional chemical data based on fingerprints and similarity measurements. *Journal of Mathematical Chemistry*, 40(1):15–27, July 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9118-5`.

Bayon:2006:ONE

[1080] L. Bayón, J. M. Grau, M. M. Ruiz, and P. M. Suárez. Optimization of SO_2 and NO_x emissions in thermal plants. *Journal of Mathematical Chemistry*, 40(1):29–41, July 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9127-4`.

Levitina:2006:FDF

[1081] T. Levitina and E. J. Brändas. Filter diagonalization with finite Fourier transform eigenfunctions. *Journal of Mathematical Chemistry*, 40(1):43–47, July 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9124-7`.

Alonso:2006:ASN

[1082] P. Alonso, R. Cortina, I. Díaz, and J. Ranilla. Analyzing scalability of Neville elimination. *Journal of Mathematical Chemistry*, 40(1):49–61, July 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9125-6`.

Garcia:2006:NHT

[1083] M. Ángeles Pérez García. The Nosé-Hoover thermostat in molecular dynamics for nuclear matter. *Journal of Mathematical Chemistry*, 40 (1):63–69, July 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9120-y`.

Vigo-Aguiar:2006:NEO

[1084] Jesús Vigo-Aguiar and Higinio Ramos. A new eighth-order A-stable method for solving differential systems arising in chemical reactions. *Journal of Mathematical Chemistry*, 40(1):71–83, July 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9121-x`.

Belkic:2006:MOV

[1085] Dzevad Belkić and Karen Belkić. Mathematical optimization of in vivo NMR chemistry through the fast Padé transform: Potential relevance for early breast cancer detection by magnetic resonance spectroscopy. *Journal of Mathematical Chemistry*, 40(1):85–103, July 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9123-8`.

Nicholson:2006:TS

[1086] Victor A. Nicholson. Twisted surfaces. *Journal of Mathematical Chemistry*, 40(2):105–117, August 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9004-6`.

Snyder:2006:MVC

[1087] Victor A. Snyder. Mass variables and chemical potentials in the Gibbs and De Donder formulations of chemical equilibrium. *Journal of Mathematical Chemistry*, 40(2):119–134, August 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9016-2`.

Liu:2006:RIU

[1088] Huiqing Liu, Xiangfeng Pan, and Jun-Ming Xu. On the Randić index of unicyclic conjugated molecules. *Journal of Mathematical Chemistry*, 40(2):135–143, August 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9017-1`.

Wang:2006:LSC

[1089] Lijie Wang, Liqin Wang, Shigeru Arimoto, and Paul G. Mezey. Large-scale chirality measures and general symmetry deficiency measures for functional group polyhedra of proteins. *Journal of Mathematical Chemistry*, 40(2):145–153, August 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9019-z`.

Veljan:2006:AMG

[1090] Darko Veljan and Damir Vukicević. On acyclic molecular graphs with prescribed numbers of edges that connect vertices with given degrees. *Journal of Mathematical Chemistry*, 40(2):155–178, August 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9021-5`.

Guseinov:2006:EBF

[1091] I. I. Guseinov and B. A. Mamedov. Evaluation of the Boys function using analytical relations. *Journal of Mathematical Chemistry*, 40(2): 179–183, August 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9023-3`.

Ji:2006:TCN

[1092] Ming Ji and Chun Li. TB-curve, a new 2-D graphical representation of DNA sequences. *Journal of Mathematical Chemistry*, 40(2):185–193, August 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9063-3`.

Simos:2006:P

[1093] T. E. Simos. Preface. *Journal of Mathematical Chemistry*, 40(3):195, October 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-006-9162-1; http://link.springer.com/article/10.1007/s10910-006-9162-1`.

Begue:2006:SPM

[1094] Didier Begue, Neil Gohaud, Ross Brown, and Claude Pouchan. An single program multiple data strategy for calculation of anharmonic vibrations. *Journal of Mathematical Chemistry*, 40(3):197–211, October 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9163-0`.

Garcia:2006:CCD

[1095] Gonzalo Cerruela García, Irene Luque Ruiz, and Miguel Ángel Gómez-Nieto. Clustering of chemical databases by means of the projection of maximum overlapping sets similarity measurements onto multidimensional spaces. *Journal of Mathematical Chemistry*, 40(3):213–231, October 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9164-z`.

Haskopoulos:2006:IDM

[1096] Anastasios Haskopoulos and George Maroulis. Interaction dipole moment in Rg–Xe (Rg = He, Ne, Ar, and Kr) heterodiatoms from conventional ab initio and density functional theory calculations. *Journal of Mathematical Chemistry*, 40(3):233–241, October 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9165-y`.

Hua:2006:NSG

[1097] Wei Hua, Xueshen Liu, and Peizhu Ding. Numerical solution for the Gross–Pitaevskii equation. *Journal of Mathematical Chemistry*, 40(3): 243–255, October 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9166-x`.

Monovasilis:2006:TFE

[1098] Th. Monovasilis, Z. Kalogiratou, Th. Monovasilis, and T. E. Simos. Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 40(3):257–267, October 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9167-9`.

Psihoyios:2006:NSR

[1099] G. Psihoyios and T. E. Simos. The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order predictor–corrector methods. *Journal of Mathematical Chemistry*, 40(3):269–293, October 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9168-8`.

Romiszowski:2006:PSB

[1100] Piotr Romiszowski and Andrzej Sikorski. Properties of star-branched and linear chains in confined space: a computer simulation study. *Journal of Mathematical Chemistry*, 40(3):295–303, October 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9169-7`.

Simos:2006:FSE

[1101] T. E. Simos. A four-step exponentially fitted method for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 40(3):305–318, October 2006. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9170-1.

Wu:2006:ESO

[1102] Ming-Hu Wu and Wei-Dong Zou. Electronic structure of the organic half-metallic magnet: 2-(5-pyrimidinyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-3-oxoimidazol-1-oxyl. *Journal of Mathematical Chemistry*, 40(3): 319–325, October 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9171-0.

Bucknum:2006:TFSb

[1103] Michael J. Bucknum and Eduardo A. Castro. On topological form in structures. *Journal of Mathematical Chemistry*, 40(4):327–340, November 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9160-3.

Bucknum:2006:DEC

[1104] Michael J. Bucknum and Eduardo A. Castro. Dynamic elasticity of cubic diamond. *Journal of Mathematical Chemistry*, 40(4):341–347, November 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-9038-9.

Francisco:2006:DBG

[1105] Juliano B. Francisco, José Mario Martínez, and Leandro Martínez. Density-based globally convergent trust-region methods for self-consistent field electronic structure calculations. *Journal of Mathematical Chemistry*, 40(4):349–377, November 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9058-0.

Lu:2006:NLI

[1106] Chunhui Lu, Weimin Guo, Xiaofang Hu, Yang Wang, and Chunsheng Yin. A novel Lu index to QSPR studies of aldehydes and ketones. *Journal of Mathematical Chemistry*, 40(4):379–388, November 2006. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9055-3.

Dey:2007:FMM

[1107] Bijoy K. Dey, Stuart Bothwell, and Paul W. Ayers. Fast marching method for calculating reactive trajectories for chemical reactions. *Jour-*

nal of Mathematical Chemistry, 41(1):1–25, January 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9060-6`.

Wagniere:2007:CTC

[1108] Georges H. Wagnière. On the chirality of torus curves and knots. *Journal of Mathematical Chemistry*, 41(1):27–31, January 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9086-9`.

Yu:2007:MSI

[1109] Aimei Yu and Xuezheng Lv. The Merrifield–Simmons indices and Hosoya indices of trees with k pendant vertices. *Journal of Mathematical Chemistry*, 41(1):33–43, January 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9088-7`.

Liu:2007:SUB

[1110] Huiqing Liu, Mei Lu, and Feng Tian. Some upper bounds for the energy of graphs. *Journal of Mathematical Chemistry*, 41(1):45–57, January 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9183-9`.

Karimi:2007:EMC

[1111] Sasan Karimi, Marty Lewinter, and Sudesh Kalyanswamy. On the equitability of multiply-connected monolayered cyclofusene. *Journal of Mathematical Chemistry*, 41(1):59–61, January 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9192-8`.

Deng:2007:PIP

[1112] Hanyuan Deng, Shubo Chen, and Jie Zhang. The PI index of phenylenes. *Journal of Mathematical Chemistry*, 41(1):63–69, January 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9198-2`.

Berberan-Santos:2007:COS

[1113] Mário N. Berberan-Santos. Computation of one-sided probability density functions from their cumulants. *Journal of Mathematical Chemistry*, 41(1):71–77, January 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9069-x`.

Anastassi:2007:FEF

[1114] Z. A. Anastassi and T. E. Simos. A family of exponentially-fitted Runge–Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 41 (1):79–100, January 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9071-3`.

Kardos:2007:TF

[1115] Frantisek Kardos. Tetrahedral fulleroids. *Journal of Mathematical Chemistry*, 41(2):101–111, February 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9057-1`.

Liu:2007:CDH

[1116] Shi-Xing Liu, Ya-Qiu Lang, Xue-Shen Liu, Pei-Zhu Ding, and Yue-Ying Qi. Classical dynamics of H_2^+ in an intense laser field by using the symplectic method. *Journal of Mathematical Chemistry*, 41(2): 113–122, February 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9059-z`.

Zhang:2007:UBC

[1117] Heping Zhang and Dong Ye. An upper bound for the Clar number of fullerene graphs. *Journal of Mathematical Chemistry*, 41(2): 123–133, February 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9061-5`.

Lim:2007:AER

[1118] Teik-Cheng Lim. Application of extended-Rydberg parameters for extracting the 2-body portion of Kaxiras–Pandey function. *Journal of Mathematical Chemistry*, 41(2):135–142, February 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9062-4`.

Xu:2007:FSL

[1119] Xiufang Xu, Guichang Wang, Xuezhuang Zhao, Yinming Pan, Yunxiao Liang, and Zhenfeng Shang. Fuzzy symmetries for linear molecules and their molecular orbitals. *Journal of Mathematical Chemistry*, 41(2): 143–160, February 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9065-1`.

Zhang:2007:MRI

[1120] Lian-Zhu Zhang, Mei Lu, and Feng Tian. Maximum Randić index on trees with k-pendant vertices. *Journal of Mathematical Chemistry*, 41(2): 161–171, February 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9066-0`.

Hua:2007:UGM

[1121] Hongbo Hua and Hanyuan Deng. On unicycle graphs with maximum and minimum zeroth-order general Randić index. *Journal of Mathematical Chemistry*, 41(2):173–181, February 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9067-z`.

Doslic:2007:FGE

[1122] Tomislav Doslić. Fullerene graphs with exponentially many perfect matchings. *Journal of Mathematical Chemistry*, 41(2):183–192, February 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9068-y`.

Duchowicz:2007:NMD

[1123] Pablo R. Duchowicz, Michael J. Bucknum, and Eduardo A. Castro. New molecular descriptors based upon the Euler equations for chemical graphs. *Journal of Mathematical Chemistry*, 41(2):193–208, February 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9070-4`.

Carbo-Dorca:2007:EPR

[1124] Ramon Carbó-Dorca. On Einstein–Podolsky–Rosen paradox. *Journal of Mathematical Chemistry*, 41(3):209–215, April 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9054-4`.

Doslic:2007:GFN

[1125] Tomislav Doslić. Global forcing number of benzenoid graphs. *Journal of Mathematical Chemistry*, 41(3):217–229, April 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9056-2`.

Arimoto:2007:RST

[1126] Shigeru Arimoto. Repeat space theory applied to carbon nanotubes and related molecular networks. I. *Journal of Mathematical Chemistry*, 41 (3):231–269, April 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9064-2`.

Li:2007:HTS

[1127] Songjun Li, Wuke Li, Xiao Hao, Pingchu Chen, and Guangfu Yang. High-throughput screening: Establishing mathematical and physical models for bio-target immobilization. *Journal of Mathematical Chemistry*, 41 (3):271–282, April 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9073-1`.

Bodroza-Pantic:2007:ASC

[1128] Olga Bodroza-Pantić. Algebraic structure count of some cyclic hexagonal-square chains on the Möbius strip. *Journal of Mathematical Chemistry*, 41(3):283–294, April 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9074-0`.

DeLeenheer:2007:MCR

[1129] Patrick De Leenheer, David Angeli, and Eduardo D. Sontag. Monotone chemical reaction networks. *Journal of Mathematical Chemistry*, 41 (3):295–314, April 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9075-z`.

Darafsheh:2007:FNR

[1130] M. R. Darafsheh, Y. Farjami, A. R. Ashrafi, and M. Hamadanian. Full non-rigid group of sponge and pina. *Journal of Mathematical Chemistry*, 41(3):315–326, April 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9076-y`.

Marmorino:2007:CIW

[1131] M. G. Marmorino. Comment: Improvement of Weyl's Inequality. *Journal of Mathematical Chemistry*, 41(3):327, April 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-006-9072-2; http://link.springer.com/article/10.1007/s10910-006-9072-2`. See [1009].

Ikhdair:2007:BEE

[1132] Sameer M. Ikhdair and Ramazan Sever. Bound energy for the exponential–cosine-screened Coulomb potential. *Journal of Mathematical Chemistry*, 41(4):329–341, May 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9080-2`.

Ikhdair:2007:BSM

[1133] Sameer M. Ikhdair and Ramazan Sever. Bound states of a more general exponential screened Coulomb potential. *Journal of Mathematical Chemistry*, 41(4):343–353, May 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9226-x`.

Ivanciuc:2007:PCE

[1134] Teodora Ivanciuc, Douglas J. Klein, and Ovidiu Ivanciuc. Posetic cluster expansion for substitution-reaction networks and application to methylated cyclobutanes. *Journal of Mathematical Chemistry*, 41(4):355–379, May 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9077-x`.

Lim:2007:AMC

[1135] Teik-Cheng Lim. On the applicability of mathematical constants and sequences in intermolecular potential energy functions. *Journal of Mathematical Chemistry*, 41(4):381–391, May 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9084-y`.

Garcia-Molina:2007:FSK

[1136] F. García-Molina, J. L. Muñoz, P. A. García-Ruíz, J. N. Rodríguez-López, F. García-Cánovas, J. Tudela, and R. Varón. A further step in the kinetic characterisation of the tyrosinase enzymatic system. *Journal of Mathematical Chemistry*, 41(4):393–406, May 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9082-0`.

Taseli:2007:LPM

[1137] H. Taseli and H. Alici. The Laguerre pseudospectral method for the reflection symmetric Hamiltonians on the real line. *Journal of Mathematical Chemistry*, 41(4):407–416, May 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9083-z`.

Luzanov:2007:SOE

[1138] A. V. Luzanov and Dmitry Nerukh. Simple one-electron invariants of molecular chirality. *Journal of Mathematical Chemistry*, 41(4):417–435, May 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9087-8`.

Belkic:2007:DRM

[1139] Dzevad Belkić and Karen Belkić. Decisive role of mathematical methods in early cancer diagnostics: optimized Padé-based magnetic resonance spectroscopy. *Journal of Mathematical Chemistry*, 42(1):1–35, July 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9227-9`.

John:2007:MCP

[1140] Peter E. John, Padmakar V. Khadikar, and Jyoti Singh. A method of computing the PI index of benzenoid hydrocarbons using orthogonal cuts. *Journal of Mathematical Chemistry*, 42(1):37–45, July 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9100-2`.

Liao:2007:SDP

[1141] Bo Liao, Renfa Li, Wen Zhu, and Xuyu Xiang. On the similarity of DNA primary sequences based on 5-D representation. *Journal of Mathematical Chemistry*, 42(1):47–57, July 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9091-z`.

Bochevarov:2007:SSR

[1142] Arteum D. Bochevarov and C. David Sherrill. Some simple results following from Löwdin's partitioning technique. *Journal of Mathematical Chemistry*, 42(1):59–64, July 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9097-6`.

Li:2007:CST

[1143] Xianyue Li and Heping Zhang. Characterizations for some types of DNA graphs. *Journal of Mathematical Chemistry*, 42(1):65–79, July 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9099-4`.

Hao:2007:EDG

[1144] Jianxiu Hao. Estimate the distance of genome rearrangements by reversals. *Journal of Mathematical Chemistry*, 42(1):81–92, July 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9095-8`.

Lim:2007:CPG

[1145] Teik-Cheng Lim. Combination of pi and Golden Ratio in Lennard-Jones-type and Morse-type potential energy functions. *Journal of Mathematical Chemistry*, 42(1):93–101, July 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9101-1`.

Gutman:2007:GWI

[1146] Ivan Gutman, Weigen Yan, Yeong-Nan Yeh, and Bo-Yin Yang. Generalized Wiener indices of zigzagging pentachains. *Journal of Mathematical Chemistry*, 42(2):103–117, August 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9078-9`.

Wang:2007:UGM

[1147] Hongzhuan Wang and Hanyuan Deng. Unicycle graphs with maximum generalized topological indices. *Journal of Mathematical Chemistry*, 42 (2):119–124, August 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9027-z`.

Zeng:2007:EPC

[1148] Yanqiu Zeng and Fuji Zhang. Extremal polyomino chains on k-matchings and k-independent sets. *Journal of Mathematical Chemistry*, 42(2): 125–140, August 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9039-8`.

Ivanov:2007:SCP

[1149] Al. Ivanov. The structure of chemical particles. *Journal of Mathematical Chemistry*, 42(2):141–152, August 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9044-y`.

Sauerbrei:2007:DC

[1150] S. Sauerbrei and P. J. Plath. Diffusion without constraints. *Journal of Mathematical Chemistry*, 42(2):153–175, August 2007. CODEN JM-

CHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9085-x.

Guseinov:2007:COS

[1151] I. I. Guseinov. Combined open shell Hartree–Fock theory of atomic-molecular and nuclear systems. *Journal of Mathematical Chemistry*, 42 (2):177–189, August 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9090-0. See comment [1455].

Ivanauskas:2007:DRR

[1152] Feliksas Ivanauskas, Aivaras Kareiva, and Bogdan Lapcun. Diffusion and reaction rates of the yttrium aluminium garnet synthesis using different techniques. *Journal of Mathematical Chemistry*, 42(2):191–199, August 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9092-y.

Ozdogan:2007:UTA

[1153] Telhat Özdogan. Unified treatment for arbitrary-rank Cartesian electric and magnetic multipole moment operators. *Journal of Mathematical Chemistry*, 42(2):201–214, August 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9093-x.

Fujita:2007:SDC

[1154] Shinsaku Fujita. Sphericities of double cosets, double coset representations, and Fujita's proligand method for combinatorial enumeration of stereoisomers. *Journal of Mathematical Chemistry*, 42(2):215–263, August 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9094-9.

Zhao:2007:FDS

[1155] Xuezhuang Zhao, Xiufang Xu, Guichang Wang, Yinming Pan, Zhenfeng Shang, and Ruifang Li. The fuzzy d2h-symmetries of ethylene tetrahalide molecules and their molecular orbitals. *Journal of Mathematical Chemistry*, 42(2):265–288, August 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9098-5.

Faridfathi:2007:SSP

[1156] Gholamreza Faridfathi and Ramazan Sever. Supersymmetric solutions of PT-/non-PT-symmetric and non-Hermitian screened Coulomb poten-

tial via Hamiltonian hierarchy inspired variational method. *Journal of Mathematical Chemistry*, 42(3):289–296, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9081-1`.

Lu:2007:RIQ

[1157] Mei Lu and Jinwu Gao. On the Randić index of quasi-tree graphs. *Journal of Mathematical Chemistry*, 42(3):297–310, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9089-6`.

Wang:2007:UGP

[1158] Wen-Huan Wang, An Chang, and Dong-Qiang Lu. Unicyclic graphs possessing Kekulé structures with minimal energy. *Journal of Mathematical Chemistry*, 42(3):311–320, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9096-7`.

Baronas:2007:CMB

[1159] R. Baronas, F. Ivanauskas, and J. Kulys. Computational modelling of the behaviour of potentiometric membrane biosensors. *Journal of Mathematical Chemistry*, 42(3):321–336, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9102-0`.

Oztekin:2007:OIB

[1160] Emin Öztekin and Selda Özcan. Overlap integrals between irregular solid harmonics and STOs via the Fourier transform methods. *Journal of Mathematical Chemistry*, 42(3):337–351, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9104-y`.

Viswanathan:2007:NBO

[1161] Balakrishnan Viswanathan, Christopher J. Barden, and Russell J. Boyd. A non–Born–Oppenheimer self-consistent field method. *Journal of Mathematical Chemistry*, 42(3):353–365, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9105-x`.

Bucknum:2007:SCM

[1162] Michael J. Bucknum and Eduardo A. Castro. Some comments on the matter wave–light wave hypothesis. *Journal of Mathematical Chemistry*, 42(3):367–372, October 2007. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9106-9`.

Bucknum:2007:SCT

[1163] Michael J. Bucknum and Eduardo A. Castro. Some comments on the topological features of some 3-, 4-connected networks and their relationships with the numbers e and π. *Journal of Mathematical Chemistry*, 42 (3):373–376, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9107-8`.

Indulal:2007:ESN

[1164] G. Indulal and A. Vijayakumar. Energies of some non-regular graphs. *Journal of Mathematical Chemistry*, 42(3):377–386, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9108-7`.

Tezcan:2007:ESS

[1165] Cevdet Tezcan and Ramazan Sever. Exact solutions of the Schrödinger equation with position-dependent effective mass via general point canonical transformation. *Journal of Mathematical Chemistry*, 42(3):387–395, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9109-6`.

Szmytkowski:2007:RDR

[1166] Radosław Szmytkowski. Recurrence and differential relations for spherical spinors. *Journal of Mathematical Chemistry*, 42(3):397–413, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9110-0`.

Guseinov:2007:EFT

[1167] I. I. Guseinov. Expansion formulae for two-center integer and noninteger n STO charge densities and their use in evaluation of multi-center integrals. *Journal of Mathematical Chemistry*, 42(3):415–422, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9111-z`.

Ou:2007:EUM

[1168] Jianping Ou. On extremal unicyclic molecular graphs with prescribed girth and minimal Hosoya index. *Journal of Mathematical Chemistry*, 42 (3):423–432, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9112-y.

Khadikar:2007:TEA

[1169] Padmakar V. Khadikar, Jyoti Singh, and Maya Ingle. Topological estimation of aromatic stabilities of polyacenes and helicenes: Modeling of resonance energy and benzene character. *Journal of Mathematical Chemistry*, 42(3):433–446, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9113-x.

Sanchez:2007:MMR

[1170] O. Sánchez, H. Herrero, S. Hoyas, and A. E. Mucientes. Mathematical modeling of Ru(VI)-catalyzed oxidation of alcohols by hexacyanoferrate(III). *Journal of Mathematical Chemistry*, 42(3):447–459, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9114-9.

Ikhdair:2007:AEE

[1171] Sameer M. Ikhdair and Ramazan Sever. Approximate eigenvalue and eigenfunction solutions for the generalized Hulthén potential with any angular momentum. *Journal of Mathematical Chemistry*, 42(3):461–471, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9115-8.

Wang:2007:OCG

[1172] Xiaoxia Wang and Xiaofeng Guo. On the ordering of a class of graphs with respect to their matching numbers. *Journal of Mathematical Chemistry*, 42(3):473–480, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9117-6.

Fujita:2007:GTF

[1173] Shinsaku Fujita. Group-theoretical foundations for the concept of mandalas as diagrammatical expressions for characterizing symmetries of stereoisomers. *Journal of Mathematical Chemistry*, 42(3):481–534, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9128-3.

Monovasilis:2007:NSO

[1174] Th. Monovasilis and T. E. Simos. New second-order exponentially and trigonometrically fitted symplectic integrators for the numerical solution of the time-independent Schrödinger equation. *Journal of Mathematical Chemistry*, 42(3):535–545, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9129-2`.

Cai:2007:PSM

[1175] Junmeng Cai and Liqun Ji. Pattern search method for determination of DAEM kinetic parameters from nonisothermal TGA data of biomass. *Journal of Mathematical Chemistry*, 42(3):547–553, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9130-9`.

Chen:2007:EGR

[1176] Shubo Chen and Hanyuan Deng. Extremal $(n, n+1)$-graphs with respect to zeroth-order general Randić index. *Journal of Mathematical Chemistry*, 42(3):555–564, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9131-8`.

Yan:2007:SBS

[1177] Zheng Yan, Huiqing Liu, and Heguo Liu. Sharp bounds for the second Zagreb index of unicyclic graphs. *Journal of Mathematical Chemistry*, 42 (3):565–574, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9132-7`.

Vukieevic:2007:AFN

[1178] Damir Vukieević and Nenad Trinajstić. On the anti-forcing number of benzenoids. *Journal of Mathematical Chemistry*, 42(3):575–583, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9133-6`.

Berberan-Santos:2007:EPD

[1179] Mário N. Berberan-Santos. Expressing a probability density function in terms of another PDF: A generalized Gram–Charlier expansion. *Journal of Mathematical Chemistry*, 42(3):585–594, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9134-5`.

Liu:2007:GRR

[1180] Liwei Liu and Tianming Wang. On 3D graphical representation of RNA secondary structures and their applications. *Journal of Mathematical Chemistry*, 42(3):595–602, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9135-4`.

Howard:2007:ESM

[1181] I. A. Howard, C. Amovilli, N. Gidopoulos, and N. H. March. Exactly solvable model mimicking the H_2 molecule in the limit of large nuclear masses. *Journal of Mathematical Chemistry*, 42(3):603–615, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9136-3`.

Lijnen:2007:UGR

[1182] Erwin Lijnen, Arnout Ceulemans, Patrick W. Fowler, and Michel Deza. The undecakisicosahedral group and a 3-regular carbon network of genus 26. *Journal of Mathematical Chemistry*, 42(3):617–644, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9137-2`.

Huang:2007:NCB

[1183] Xuncheng Huang and Lemin Zhu. A note on competition in the bioreactor with toxin. *Journal of Mathematical Chemistry*, 42(3):645–659, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9140-7`.

Gal:2007:MFD

[1184] Tamás Gál. The mathematics of functional differentiation under conservation constraint. *Journal of Mathematical Chemistry*, 42(3):661–676, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9216-4`.

Mamedov:2007:EGE

[1185] B. A. Mamedov, Z. Merdan, and I. M. Askerov. Evaluation of generalized exponential integrals using multinomial expansion theorems. *Journal of Mathematical Chemistry*, 42(3):677, October 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.`

1007/s10910-006-9202-x; http://link.springer.com/article/10.1007/s10910-006-9202-x.

Ren:2007:DHCa

[1186] Haizhen Ren and Fuji Zhang. Double hexagonal chains with maximal Hosoya index and minimal Merrifield–Simmons index. *Journal of Mathematical Chemistry*, 42(4):679–690, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-005-9024-2.

Gabarro-Arpa:2007:CPM

[1187] Jacques Gabarro-Arpa. A central partition of molecular conformational space. III. Combinatorial determination of the volume spanned by a molecular system. *Journal of Mathematical Chemistry*, 42(4):691–706, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9079-8.

Heiberg-Andersen:2007:SCC

[1188] H. Heiberg-Andersen and A. T. Skjeltorp. Spectra of conic carbon radicals. *Journal of Mathematical Chemistry*, 42(4):707–727, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9103-z.

Li:2007:UCM

[1189] Xueliang Li, Jianbin Zhang, and Bo Zhou. On unicyclic conjugated molecules with minimal energies. *Journal of Mathematical Chemistry*, 42(4):729–740, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9116-7.

Hasanov:2007:RBC

[1190] Alemdar Hasanov and Safak Hasanoglu. Relationship between current response and time in ion transport problem including diffusion and convection. 1. an analytical approach. *Journal of Mathematical Chemistry*, 42(4):741–751, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9138-1.

Fuentes:2007:KAM

[1191] M. E. Fuentes, E. Valero, M. García-Moreno, E. Vique, and R. Varón. Kinetic analysis of the mechanism of plasminogen activation by streptokinase. *Journal of Mathematical Chemistry*, 42(4):753–774, November

2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9139-0`.

Li:2007:SUG

[1192] Xueliang Li, Jianbin Zhang, and Bo Zhou. The spread of unicyclic graphs with given size of maximum matchings. *Journal of Mathematical Chemistry*, 42(4):775–788, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9141-6`.

Varon:2007:AAE

[1193] R. Varón, M. Garcia-Moreno, J. Masiá-Pérez, F. García-Molina, F. García-Cánovas, E. Arias, E. Arribas, and F. García-Sevilla. An alternative analysis of enzyme systems based on the whole reaction time: evaluation of the kinetic parameters and initial enzyme concentration. *Journal of Mathematical Chemistry*, 42(4):789–813, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9142-5`.

Kwiatkowski:2007:ENC

[1194] Mirosław Kwiatkowski. Employing the new computer LBET class models with multivariant fitting to the analysis of single and double adsorption isotherms generated by the selected classical equations in different relative pressures. *Journal of Mathematical Chemistry*, 42(4): 815–835, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9143-4`.

Sun:2007:DBM

[1195] Shulin Sun and Lansun Chen. Dynamic behaviors of Monod type chemostat model with impulsive perturbation on the nutrient concentration. *Journal of Mathematical Chemistry*, 42(4):837–847, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9144-3`.

Hao:2007:ARM

[1196] Jianxiu Hao. An algorithm for reversal median problem. *Journal of Mathematical Chemistry*, 42(4):849–857, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9145-2`.

Jesudason:2007:MHDa

[1197] Christopher G. Jesudason. Model hysteresis dimer molecule I: Equilibrium properties. *Journal of Mathematical Chemistry*, 42(4):859–891, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9146-1`.

Jesudason:2007:MHDb

[1198] Christopher G. Jesudason. Model hysteresis dimer molecule II: deductions from probability profile due to system coordinates. *Journal of Mathematical Chemistry*, 42(4):893–908, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9147-0`.

Brinkmann:2007:FBP

[1199] Gunnar Brinkmann, Christian Grothaus, and Ivan Gutman. Fusenes and benzenoids with perfect matchings. *Journal of Mathematical Chemistry*, 42(4):909–924, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9148-z`.

Kumar:2007:AGT

[1200] Vipin Kumar and A. K. Madan. Application of graph theory: Models for prediction of carbonic anhydrase inhibitory activity of sulfonamides. *Journal of Mathematical Chemistry*, 42(4):925–940, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9149-y`.

Zhang:2007:SOR

[1201] Jie Zhang, Hanyuan Deng, and Shubo Chen. Second order Randić index of phenylenes and their corresponding hexagonal squeezes. *Journal of Mathematical Chemistry*, 42(4):941–947, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9150-5`.

Cai:2007:NOD

[1202] Junmeng Cai, Fang He, and Fusheng Yao. Nonisothermal nth-order DAEM equation and its parametric study — use in the kinetic analysis of biomass pyrolysis. *Journal of Mathematical Chemistry*, 42(4):949–956, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9151-4`.

Wang:2007:RGP

[1203] Shou-Zhong Wang and Rong Si Chen. Regular generalized polyomino graphs. *Journal of Mathematical Chemistry*, 42(4):957–967, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9152-3`.

Navarro-Laboulais:2007:TRM

[1204] J. Navarro-Laboulais, F. López, J. I. Torregrosa, S. C. Cardona, and A. Abad. Transient response, model structure and systematic errors in hybrid respirometers: structural identifiability analysis based on OUR and DO measurements. *Journal of Mathematical Chemistry*, 42(4):969–990, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9153-2`.

Guseinov:2007:UTC

[1205] I. I. Guseinov. Unified treatment of complete orthonormal sets of functions in coordinate, momentum and four-dimensional spaces and their expansion and one-range addition theorems. *Journal of Mathematical Chemistry*, 42(4):991–1001, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9154-1`.

Bielinska-Waz:2007:SSU

[1206] Dorota Bielińska-Waz, Piotr Waz, and Subhash C. Basak. Similarity studies using statistical and genetical methods. *Journal of Mathematical Chemistry*, 42(4):1003–1013, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9155-0`.

Liao:2007:FDR

[1207] Bo Liao, Wen Zhu, and Pengcheng Li. On a four-dimensional representation of RNA secondary structures. *Journal of Mathematical Chemistry*, 42(4):1015–1022, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9156-z`.

Abbas:2007:TDI

[1208] A. Abbas and A. Bouabdellah. Theoretical description of the interactions between a mixture of vapors and a set of chemical sensors by variable temperature. *Journal of Mathematical Chemistry*, 42(4):1023–1030, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (elec-

tronic). URL http://link.springer.com/article/10.1007/s10910-006-9157-y.

Yousefi:2007:EEW

[1209] Shahram Yousefi and Ali Reza Ashrafi. An exact expression for the Wiener index of a $TUC_4C_8(R)$ nanotorus. *Journal of Mathematical Chemistry*, 42(4):1031–1039, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9158-x.

Ren:2007:DHCb

[1210] Haizhen Ren and Fuji Zhang. Double hexagonal chains with minimal total π-electron energy. *Journal of Mathematical Chemistry*, 42(4):1041–1056, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9159-9.

Lin:2007:LET

[1211] Wenshui Lin and Xiaofeng Guo. On the largest eigenvalues of trees with perfect matchings. *Journal of Mathematical Chemistry*, 42(4):1057–1067, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9161-2.

Naujikas:2007:MEP

[1212] R. Naujikas, A. Malinauskas, and F. Ivanauskas. Modeling of electrocatalytic processes at conducting polymer modified electrodes. *Journal of Mathematical Chemistry*, 42(4):1069–1084, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9172-z.

Fenstad:2007:DHP

[1213] Jo Fenstad. Deciphering the hidden Pascal code of Guggenheim's quasi-chemical model. Overcoming computational limitations by use of Pascal's triangle. *Journal of Mathematical Chemistry*, 42(4):1085–1100, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9262-6.

Edgal:2007:PNN

[1214] Uduzei F. Edgal. Partial nearest neighbor PDF for multi-component material systems. *Journal of Mathematical Chemistry*, 42(4):1101–1134, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9291-1.

Mincheva:2007:NPS

[1215] Maya Mincheva and David Siegel. Nonnegativity and positiveness of solutions to mass action reaction-diffusion systems. *Journal of Mathematical Chemistry*, 42(4):1135–1145, November 2007. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9292-0.

Ivanov:2008:ETU

[1216] Al. Ivanov. Energy-time uncertainty relations and time operators. *Journal of Mathematical Chemistry*, 43(1):1–11, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9173-y.

Zhang:2008:TOR

[1217] Jie Zhang and Hanyuan Deng. Third order Randić index of phenylenes. *Journal of Mathematical Chemistry*, 43(1):12–18, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9174-x.

Deng:2008:PIP

[1218] Hanyuan Deng and Shubo Chen. PI indices of pericondensed benzenoid graphs. *Journal of Mathematical Chemistry*, 43(1):19–25, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9175-9.

Li:2008:SAD

[1219] Chun Li and Jun Wang. Similarity analysis of DNA sequences based on the generalized LZ complexity of (0,1)-sequences. *Journal of Mathematical Chemistry*, 43(1):26–31, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9176-8.

Clark:2008:EGR

[1220] Lane Clark and Ivan Gutman. The exponent in the general Randić index. *Journal of Mathematical Chemistry*, 43(1):32–44, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9177-7.

Shiu:2008:CCR

[1221] Wai Chee Shiu and Heping Zhang. A complete characterization for k-resonant Klein-bottle polyhexes. *Journal of Mathematical Chemistry*, 43

(1):45–59, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9178-6.

Tang:2008:GFT

[1222] Zikai Tang and Hanyuan Deng. The (n,n)-graphs with the first three extremal Wiener indices. *Journal of Mathematical Chemistry*, 43(1): 60–74, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9179-5.

Deng:2008:MSI

[1223] Hanyuan Deng, Shubo Chen, and Jie Zhang. The Merrifield–Simmons index in $(n, n+1)$-graphs. *Journal of Mathematical Chemistry*, 43(1): 75–91, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9180-z.

Aktas:2008:EMS

[1224] Metin Aktas and Ramazan Sever. Effective mass Schrödinger equation for exactly solvable class of one-dimensional potentials. *Journal of Mathematical Chemistry*, 43(1):92–100, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9181-y.

Flach:2008:LCP

[1225] E. H. Flach, J. Norbury, and S. Schnell. Limit cycles in the presence of convection: a first-order analysis. *Journal of Mathematical Chemistry*, 43 (1):101–110, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9182-x.

Bultinck:2008:PME

[1226] Patrick Bultinck, Marcos Mandado, and Ricardo Mosquera. The pseudo-π method examined for the computation of multicenter aromaticity indices. *Journal of Mathematical Chemistry*, 43(1):111–118, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9184-8.

Deng:2008:SHI

[1227] Hanyuan Deng. The smallest Hosoya index in $(n, n+1)$-graphs. *Journal of Mathematical Chemistry*, 43(1):119–133, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-006-9186-6.

Qi:2008:NCE

[1228] Zhongbin Qi and Heping Zhang. A note on the cyclical edge-connectivity of fullerene graphs. *Journal of Mathematical Chemistry*, 43(1):134–140, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9185-7`.

Fujita:2008:CET

[1229] Shinsaku Fujita. Combinatorial enumeration of three-dimensional trees as stereochemical models of alkanes: an approach based on Fujita's proligand method and dual recognition as uninuclear and binuclear promolecules. *Journal of Mathematical Chemistry*, 43(1):141–201, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9187-5`.

Wang:2008:UGE

[1230] Hongzhuan Wang and Hongbo Hua. Unicycle graphs with extremal Merrifield–Simmons index. *Journal of Mathematical Chemistry*, 43(1):202–209, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9188-4`.

Wang:2008:SMH

[1231] Fengyan Wang, Guoping Pang, and Lansun Chen. Study of a Monod–Haldene type food chain chemostat with pulsed substrate. *Journal of Mathematical Chemistry*, 43(1):210–226, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9189-3`.

Szalay:2008:DTO

[1232] Zsófia Szalay and Péter R. Surján. Distorted s-type orbitals: the H_2^+ problem revisited. *Journal of Mathematical Chemistry*, 43(1):227–236, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9190-x`.

Taseli:2008:SVM

[1233] H. Taseli. On the special values of monic polynomials of hypergeometric type. *Journal of Mathematical Chemistry*, 43(1):237–251, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9191-9`.

Shulyk:2008:NSS

[1234] V. N. Shulyk, O. V. Klymenko, and I. B. Svir. Numerical solution of stiff ODEs describing complex homogeneous chemical processes. *Journal of Mathematical Chemistry*, 43(1):252–264, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9193-7`.

Nalewajski:2008:EBI

[1235] R. F. Nalewajski. Entropic bond indices from molecular information channels in orbital resolution: ground-state systems. *Journal of Mathematical Chemistry*, 43(1):265–284, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9194-6`.

Ayers:2008:DCE

[1236] Paul W. Ayers. The dependence on and continuity of the energy and other molecular properties with respect to the number of electrons. *Journal of Mathematical Chemistry*, 43(1):285–303, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9195-5`.

Lim:2008:PEF

[1237] Teik-Cheng Lim. Potential energy function based on the narcissus constant, its square and its cube. *Journal of Mathematical Chemistry*, 43 (1):304–313, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9196-4`.

Szakacs:2008:ISB

[1238] Péter Szakács and Péter R. Surján. Iterative solution of Bloch-type equations: stability conditions and chaotic behavior. *Journal of Mathematical Chemistry*, 43(1):314–327, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9197-3`.

Ou:2008:AMG

[1239] Jianping Ou. On acyclic molecular graphs with maximal Hosoya index, energy, and short diameter. *Journal of Mathematical Chemistry*, 43(1): 328–337, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9199-1`.

Sun:2008:CDC

[1240] Shulin Sun and Lansun Chen. Complex dynamics of a chemostat with variable yield and periodically impulsive perturbation on the substrate. *Journal of Mathematical Chemistry*, 43(1):338–349, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9200-z`.

Gonzalez:2008:EPB

[1241] María F. González, Xavier Giménez, Javier González, and Josep Maria Bofill. Effective potential, Bohm's potential plus classical potential, analysis of quantum transmission. *Journal of Mathematical Chemistry*, 43 (1):350–364, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9201-y`.

Li:2008:SRC

[1242] Huimin Li, Xiaoming Bai, and Xiao-Song Yang. Stability results on a chemical system. *Journal of Mathematical Chemistry*, 43(1):365–374, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9203-9`.

Cai:2008:EPL

[1243] Guang hui Cai. Estimation of partial linear error-in-variables models for ρ^{-}-mixing dependence data. *Journal of Mathematical Chemistry*, 43 (1):375–385, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9204-8`.

Hefferlin:2008:DVC

[1244] Ray Hefferlin. Discrete vector calculus on periodic systems of atoms and molecules. *Journal of Mathematical Chemistry*, 43(1):386–394, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9251-9`.

Belkic:2008:MMN

[1245] Dzevad Belkić and Karen Belkić. Mathematical modeling of an NMR chemistry problem in ovarian cancer diagnostics. *Journal of Mathematical Chemistry*, 43(1):395–425, January 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9279-x`.

Guseinov:2008:UCC

[1246] I. I. Guseinov. Use of Cartesian coordinates in evaluation of multicenter multielectron integrals over Slater type orbitals and their derivatives. *Journal of Mathematical Chemistry*, 43(2):427–434, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9205-7`.

Jia:2008:PDE

[1247] Chun-Sheng Jia, Liang-Zhong Yi, and Yu Sun. Position-dependent effective mass Schrödinger equations for PT-symmetric potentials. *Journal of Mathematical Chemistry*, 43(2):435–446, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9206-6`.

Sun:2008:ADB

[1248] Mingjing Sun and Lansun Chen. Analysis of the dynamical behavior for enzyme-catalyzed reactions with impulsive input. *Journal of Mathematical Chemistry*, 43(2):447–456, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9207-5`.

Wang:2008:FNT

[1249] Hongwei Wang, Dong Ye, Heping Zhang, and Hongwei Wang. The forcing number of toroidal polyhexes. *Journal of Mathematical Chemistry*, 43(2):457–475, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9208-4`.

Li:2008:MEU

[1250] Feng Li and Bo Zhou. Minimal energy of unicyclic graphs of a given diameter. *Journal of Mathematical Chemistry*, 43(2):476–484, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9209-3`.

Zhao:2008:FSA

[1251] Xuezhuang Zhao, Guichang Wang, Xiufang Xu, Yinming Pan, Ruifang Li, Zhengfeng Shang, and Zucheng Li. The fuzzy D_{6h}-symmetries of azines molecules and their molecular orbitals. *Journal of Mathematical Chemistry*, 43(2):485–507, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9210-x`.

Estrada:2008:GSS

[1252] Ernesto Estrada and Adelio R. Matamala. GTI-space: the space of generalized topological indices. *Journal of Mathematical Chemistry*, 43 (2):508–517, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9211-9`.

Zivkovic:2008:IFQ

[1253] Tomislav P. Zivković. Interaction of a finite quantum system with an infinite quantum system that contains a single one-parameter eigenvalue band. *Journal of Mathematical Chemistry*, 43(2):518–600, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9212-8`.

Wang:2008:AMH

[1254] Fengyan Wang, Guoping Pang, and Jin Hui. Analysis of a Monod–Haldene type food chain chemostat with seasonally variably pulsed input and washout. *Journal of Mathematical Chemistry*, 43(2):601–619, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9213-7`.

Duchowicz:2008:ANR

[1255] Pablo R. Duchowicz, Eduardo A. Castro, and Francisco M. Fernández. Application of a novel ranking approach in QSPR–QSAR. *Journal of Mathematical Chemistry*, 43(2):620–636, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9214-6`.

Cai:2008:DFF

[1256] Junmeng Cai and Ronghou Liu. Dependence of the frequency factor on the temperature: a new integral method of nonisothermal kinetic analysis. *Journal of Mathematical Chemistry*, 43(2):637–646, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9215-5`.

Doslic:2008:SNF

[1257] Tomislav Doslić. Saturation number of fullerene graphs. *Journal of Mathematical Chemistry*, 43(2):647–657, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9217-3`.

Arimoto:2008:RST

[1258] Shigeru Arimoto. Repeat space theory applied to carbon nanotubes and related molecular networks. II. *Journal of Mathematical Chemistry*, 43 (2):658–673, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9218-2`.

Randic:2008:RDL

[1259] Milan Randić, Jure Zupan, and Tomaz Pisanski. On representation of DNA by line distance matrix. *Journal of Mathematical Chemistry*, 43(2): 674–692, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9219-1`.

He:2008:RPR

[1260] Jianfeng He and Jing Li. The reaction probability and the reaction cross-section of the $N(^4\ S) + O_2\ (X\ ^3\Sigma_g^-) \rightarrow NO(X^2\Pi) + O(^3P)$ reaction. *Journal of Mathematical Chemistry*, 43(2):693–700, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9220-8`.

Peuker:2008:AET

[1261] Katrin Peuker and María Belén Ruiz. Analytical evaluation of three-center nuclear-attraction integrals over s-Slater orbitals for asymmetrical conformations of the centers. *Journal of Mathematical Chemistry*, 43(2): 701–712, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9221-7`.

Guo:2008:SUB

[1262] Ji-Ming Guo. Sharp upper bounds for total π-electron energy of alternant hydrocarbons. *Journal of Mathematical Chemistry*, 43(2):713–718, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9222-6`.

Vukicevic:2008:AKN

[1263] Damir Vukicević and Nenad Trinajstić. On the anti-Kekulé number and anti-forcing number of cata-condensed benzenoids. *Journal of Mathematical Chemistry*, 43(2):719–726, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9223-5`.

Wang:2008:FSL

[1264] Maolin Wang, Hongbo Hua, and Dongdong Wang. The first and second largest Merrifield–Simmons indices of trees with prescribed pendent vertices. *Journal of Mathematical Chemistry*, 43(2):727–736, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9224-4`.

Hua:2008:ZOG

[1265] Hongbo Hua, Maolin Wang, and Hongzhuan Wang. On zeroth-order general Randić index of conjugated unicyclic graphs. *Journal of Mathematical Chemistry*, 43(2):737–748, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-006-9225-3`.

Sever:2008:BSS

[1266] Ramazan Sever, Mahmut Bucurgat, Cevdet Tezcan, and Özlem Yesiltas. Bound state solution of the Schrödinger equation for Mie potential. *Journal of Mathematical Chemistry*, 43(2):749–755, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9228-8`.

Randic:2008:GBA

[1267] Milan Randić. On a geometry-based approach to protein sequence alignment. *Journal of Mathematical Chemistry*, 43(2):756–772, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9229-7`.

Balaban:2008:PEB

[1268] Alexandru T. Balaban, Milan Randić, and Damir Vukicević. Partition of π-electrons between faces of polyhedral carbon aggregates. *Journal of Mathematical Chemistry*, 43(2):773–779, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9230-1`.

Nalewajski:2008:CBT

[1269] Roman F. Nalewajski. Chemical bonds through probability scattering: Information channels for intermediate-orbital stages. *Journal of Mathematical Chemistry*, 43(2):780–830, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9231-0`.

Hua:2008:HIU

[1270] Hongbo Hua. Hosoya index of unicyclic graphs with prescribed pendent vertices. *Journal of Mathematical Chemistry*, 43(2):831–844, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9232-z`.

Sever:2008:ESS

[1271] Ramazan Sever, Cevdet Tezcan, Metin Aktas, and Özlem Yesiltas. Exact solution of Schrödinger equation for pseudoharmonic potential. *Journal of Mathematical Chemistry*, 43(2):845–851, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9233-y`.

Xu:2008:GHP

[1272] Shoujun Xu and Heping Zhang. Generalized Hosoya polynomials of hexagonal chains. *Journal of Mathematical Chemistry*, 43(2):852–863, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9234-x`.

Zhang:2008:VCA

[1273] Yi Zhang and Jun Wang. Volatilities of codons and its application in similarity analysis of biological sequences. *Journal of Mathematical Chemistry*, 43(2):864–873, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9235-9`.

Cox:2008:HLO

[1274] Mary A. Cox, Thomas S. Hughes, Joanna A. Ellis-Monaghan, and Kathleen R. Mondanaro. Hydrocarbon links in an octet truss. *Journal of Mathematical Chemistry*, 43(2):874–891, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9323-x`.

Karimi:2008:BC

[1275] Sasan Karimi, Marty Lewinter, and Sudesh Kalyanswamy. Bilayered cyclofusene. *Journal of Mathematical Chemistry*, 43(2):892–900, February 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9334-7`.

Pang:2008:SLV

[1276] Guoping Pang, Fengyan Wang, and Lansun Chen. Study of Lotka–Volterra food chain chemostat with periodically varying dilution rate. *Journal of Mathematical Chemistry*, 43(3):901–913, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9263-5`.

Cai:2008:KAS

[1277] Junmeng Cai and Ronghou Liu. Kinetic analysis of solid-state reactions: errors involved in the determination of the kinetic parameters calculated by one type of integral methods. *Journal of Mathematical Chemistry*, 43 (3):914–920, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9273-3`.

Yesiltas:2008:ETC

[1278] Özlem Yesiltas and Ramazan Sever. Exponential type complex and non-Hermitian potentials within quantum Hamilton–Jacobi formalism. *Journal of Mathematical Chemistry*, 43(3):921–931, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9238-6`.

Bai:2008:NMR

[1279] Fenglan Bai, Dachao Li, and Tianming Wang. A new mapping rule for RNA secondary structures with its applications. *Journal of Mathematical Chemistry*, 43(3):932–943, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9303-1`.

Berkdemir:2008:SIA

[1280] Cüneyt Berkdemir, Ayse Berkdemir, and Ramazan Sever. Shape-invariance approach and Hamiltonian hierarchy method on the Woods–Saxon potential for $\ell \neq 0$ states. *Journal of Mathematical Chemistry*, 43 (3):944–954, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9335-6`.

Jiang:2008:CIT

[1281] Yue Jiang and Mei Lu. On the connectivity index of trees. *Journal of Mathematical Chemistry*, 43(3):955–965, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9281-3`.

Marmorino:2008:ABS

[1282] M. G. Marmorino. Alternatives to Bazley's special choice for eigenvalue lower bounds. *Journal of Mathematical Chemistry*, 43(3):966–975, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9270-6`.

Jesudason:2008:FRC

[1283] Christopher G. Jesudason. The form of the rate constant for elementary reactions at equilibrium from MD: framework and proposals for thermokinetics. *Journal of Mathematical Chemistry*, 43(3): 976–1023, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9320-0`.

Guseinov:2008:UTCa

[1284] I. I. Guseinov. On the unified treatment of complete orthonormal sets of functions in coordinate, momentum, and four dimensional spaces and their expansion and one-range addition theorems. *Journal of Mathematical Chemistry*, 43(3):1024–1031, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9239-5`.

Volpe:2008:PCA

[1285] C. Della Volpe and S. Siboni. Principal component analysis and multicomponent surface free energy theories. *Journal of Mathematical Chemistry*, 43(3):1032–1051, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9247-5`.

Guo:2008:CDH

[1286] Jing Guo, Xueshen Liu, Bing Yan, and Peizhu Ding. Classical dynamics of 3D hydrogen molecular ion in intense laser fields. *Journal of Mathematical Chemistry*, 43(3):1052–1068, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9268-0`.

Carbo-Dorca:2008:MALa

[1287] Ramon Carbó-Dorca and Patrick Bultinck. Mathematical aspects of the LCAO MO first order density function (3): A general localization procedure. *Journal of Mathematical Chemistry*, 43(3):1069–1075, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9242-x`.

Carbo-Dorca:2008:MALb

[1288] Ramon Carbó-Dorca. Mathematical aspects of the LCAO MO first order density function (1): atomic partition, metric structure and practical applications. *Journal of Mathematical Chemistry*, 43(3):1076–1101, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9244-8`.

Carbo-Dorca:2008:MALc

[1289] Ramon Carbó-Dorca. Mathematical aspects of the LCAO MO first order density function (2): Relationships between density functions. *Journal of Mathematical Chemistry*, 43(3):1102–1118, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9245-7`.

Sanctuary:2008:IDF

[1290] B. C. Sanctuary and F. P. Temme. Indistinguishability in DR n-fold point-sets & their $\mathcal{S}_\setminus$-invariant dual projective mappings: limitations imposed on Racah–Wigner algebras for Liouville spin dynamics of $[A]_n$ X multi-invariant NMR systems. *Journal of Mathematical Chemistry*, 43 (3):1119–1126, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9236-8`.

Cai:2008:IVD

[1291] Junmeng Cai, Ronghou Liu, and Fei Shen. Improved version of Doyle integral method for nonisothermal kinetics of solid-state reactions. *Journal of Mathematical Chemistry*, 43(3):1127–1133, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9254-6`.

Lim:2008:SSR

[1292] Jisun Lim. Stability of solutions to a reaction diffusion system based upon chemical reaction kinetics. *Journal of Mathematical Chemistry*, 43 (3):1134–1140, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9255-5`.

Zhao:2008:FSP

[1293] Xuezhuang Zhao, Zhengfeng Shang, Guichang Wang, Xiufang Xu, Ruifang Li, Yinming Pan, and Zucheng Li. Fuzzy space periodic symmetries for polyynes and their cyano-compounds. *Journal of Mathematical Chemistry*, 43(3):1141–1162, March 2008. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9243-9`.

Trif:2008:MPS

[1294] Damian Trif. Matlab package for the Schrödinger equation. *Journal of Mathematical Chemistry*, 43(3):1163–1176, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9266-2`.

Yuan:2008:PIG

[1295] Chun xin Yuan, Li wei Liu, Tian ming Wang, and Chun Li. On property of the invariant of graphical representations of DNA sequences. *Journal of Mathematical Chemistry*, 43(3):1177–1183, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9267-1`.

He:2008:QCR

[1296] Jianfeng He and Jing Li. The QCT calculation of the rate constants for the $N(^4S) + O_2\ (X^3\Sigma_g^-) \rightarrow NO(X^2\Pi) + O(^3P)$ reaction. *Journal of Mathematical Chemistry*, 43(3):1184–1192, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9271-5`.

Cai:2008:IVJ

[1297] Junmeng Cai and Ronghou Liu. An improved version of Junmeng–Fang–Weiming–Fusheng approximation for the temperature integral. *Journal of Mathematical Chemistry*, 43(3):1193–1198, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9252-8`.

Liu:2008:PCC

[1298] Huiqing Liu. The proof of a conjecture concerning acyclic molecular graphs with maximal Hosoya index and diameter 4. *Journal of Mathematical Chemistry*, 43(3):1199–1206, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9256-4`.

Li:2008:RRS

[1299] Genyuan Li, Herschel Rabitz, Jishan Hu, Zheng Chen, and Yiguang Ju. Regularized random-sampling high dimensional model representation (RS-HDMR). *Journal of Mathematical Chemistry*, 43(3):1207–1232, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9250-x.

Pogliani:2008:CEH

[1300] Lionello Pogliani. Core electrons and hydrogen atoms in chemical graph theory. *Journal of Mathematical Chemistry*, 43(3):1233–1255, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9253-7.

Zhang:2008:TAA

[1301] Hong Zhang and Lansun Chen. Toxic action and antibiotic in the chemostat: permanence and extinction of a model with functional response. *Journal of Mathematical Chemistry*, 43(3):1256–1272, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9278-y.

Su:2008:GST

[1302] Houqin Su, Xuncheng Huang, Xuncheng Huang, and Xiaoning Xu. Global stability of a three-dimensional bio-reactor with inhibition responses. *Journal of Mathematical Chemistry*, 43(3):1273–1284, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9264-4.

Kwiatkowski:2008:ENC

[1303] Mirosław Kwiatkowski. Employing the new computer LBET class models with multivariant fitting to the analysis of single and double adsorption isotherms generated by the selected classical equations in different relative pressures. *Journal of Mathematical Chemistry*, 43(3):1285, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-007-9280-4; http://link.springer.com/article/10.1007/s10910-007-9280-4.

Wagniere:2008:CTC

[1304] Georges H. Wagnière. On the chirality of torus curves and knots. *Journal of Mathematical Chemistry*, 43(3):1286, March 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-007-9311-1; http://link.springer.com/article/10.1007/s10910-007-9311-1.

Bielinska-Waz:2008:CSS

[1305] Dorota Bielińska-Waz and Piotr Waz. Correlations in spectral statistics. *Journal of Mathematical Chemistry*, 43(4):1287–1300, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9241-y`.

Zawadzka:2008:ASP

[1306] Izabela K. Zawadzka, Jacek A. Soroka, Marta J. Sawicka, and Monika Gasiorowska. An attempt to separate $A \rightarrow B$ process spectra. SEparation by MInimum overLApping Method (SEMILAM). *Journal of Mathematical Chemistry*, 43(4):1301–1317, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9246-6`.

Pedersen:2008:QSS

[1307] Morten Gram Pedersen, Alberto Maria Bersani, and Enrico Bersani. Quasi steady-state approximations in complex intracellular signal transduction networks — a word of caution. *Journal of Mathematical Chemistry*, 43(4):1318–1344, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9248-4`.

Lim:2008:CBO

[1308] Teik-Cheng Lim. Connection between the Ogilvie and the Murrell–Sorbie potential energy functions. *Journal of Mathematical Chemistry*, 43(4):1345–1354, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9249-3`.

Banaji:2008:ETN

[1309] Murad Banaji and Stephen Baigent. Electron transfer networks. *Journal of Mathematical Chemistry*, 43(4):1355–1370, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9257-3`.

Pang:2008:AMT

[1310] Guoping Pang, Yanlai Liang, and Fengyan Wang. Analysis of Monod type food chain chemostat with k-times periodically pulsed input. *Journal of Mathematical Chemistry*, 43(4):1371–1388, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9258-2`.

Wang:2008:MEC

[1311] Maolin Wang, Hongbo Hua, and Dongdong Wang. Minimal energy on a class of graphs. *Journal of Mathematical Chemistry*, 43(4):1389–1402, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9259-1`.

Delgado:2008:EUC

[1312] Víctor Delgado and Rodolfo Figueroa. Existence, uniqueness, and calculation of the physically acceptable solution of a particular case of the Sherman equations. *Journal of Mathematical Chemistry*, 43(4): 1403–1421, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9260-8`.

Doslic:2008:EMC

[1313] Tomislav Doslić. On the existence of multiply connected monolayered cyclofusenes with given parameters. *Journal of Mathematical Chemistry*, 43(4):1422–1428, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9265-3`.

Zhang:2008:QAE

[1314] Chunli Zhang, Xueshen Liu, and Peizhu Ding. The quantitative analysis of enhancement of high-order harmonics in two-color intense laser fields. *Journal of Mathematical Chemistry*, 43(4):1429–1436, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9269-z`.

Berberan-Santos:2008:VWE

[1315] Mario N. Berberan-Santos, Evgeny N. Bodunov, and Lionello Pogliani. The van der Waals equation: analytical and approximate solutions. *Journal of Mathematical Chemistry*, 43(4):1437–1457, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9272-4`.

Hasanoglu:2008:RBC

[1316] Safak Hasanoglu and Arzu Erdem. Relationship between current response and time in ion transport problem including diffusion and convection. 2. Numerical approach. *Journal of Mathematical Chemistry*, 43 (4):1458–1469, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9274-2`.

Wang:2008:ATT

[1317] Fengyan Wang, Shuwen Zhang, and Guoping Pang. Analysis of a Tessiet type food chain chemostat with k-times periodically pulsed input. *Journal of Mathematical Chemistry*, 43(4):1470–1488, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9275-1`.

Baowan:2008:ELN

[1318] Duangkamon Baowan and James M. Hill. Equilibrium locations for nested carbon nanocones. *Journal of Mathematical Chemistry*, 43(4): 1489–1504, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9276-0`.

Maioli:2008:ECC

[1319] Marco Maioli, Károly Micskei, Luciano Caglioti, Claudia Zucchi, and Gyula Pályi. Evolution of chirality in consecutive asymmetric autocatalytic reaction cycles. *Journal of Mathematical Chemistry*, 43(4): 1505–1515, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9277-z`.

Ivanauskas:2008:AMC

[1320] F. Ivanauskas, I. Kaunietis, V. Laurinavicius, J. Razumiene, and R. Simkus. Apparent Michaelis constant of the enzyme modified porous electrode. *Journal of Mathematical Chemistry*, 43(4):1516–1526, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9237-7`.

Guseinov:2008:AEO

[1321] I. I. Guseinov and B. A. Mamedov. Accurate evaluation of overlap integrals of Slater type orbitals with noninteger principal quantum numbers using complete orthonormal sets of Ψ^{α}- exponential type orbitals. *Journal of Mathematical Chemistry*, 43(4):1527–1532, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9240-z`.

Zhang:2008:WAI

[1322] Tonghua Zhang, Moses O. Tadé, Yu-Chu Tian, Yanduo Zhang, and Johan Utomo. Wavelet approach incorporated with optimization for solving stiff systems. *Journal of Mathematical Chemistry*, 43(4):1533–1548,

May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9282-2.

Ruiz:2008:ASQ

[1323] Irene Luque Ruiz, Manuel Urbano-Cuadrado, and Miguel Ángel Gómez-Nieto. Approximate similarity and QSAR in the study of spirosuccinimide type aldose reductase inhibitors. *Journal of Mathematical Chemistry*, 43(4):1549–1559, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9283-1.

Bielinska-Waz:2008:SST

[1324] Dorota Bielińska-Waz, Wiesław Nowak, Lukasz Peplowski, Piotr Waz, Subhash C. Basak, and Ramanathan Natarajan. Statistical spectroscopy as a tool for the study of molecular similarity. *Journal of Mathematical Chemistry*, 43(4):1560–1572, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9284-0.

Lim:2008:ILR

[1325] Teik-Cheng Lim. Improved long range relationship between parameters of the Morse and Rydberg potential functions. *Journal of Mathematical Chemistry*, 43(4):1573–1577, May 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9285-z.

Doslic:2008:LFM

[1326] Tomislav Doslić. Leapfrog fullerenes have many perfect matchings. *Journal of Mathematical Chemistry*, 44(1):1–4, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9287-x.

King:2008:GTS

[1327] R. Bruce King. The group-theoretical structure of the atomic g shell: connection with the alternating group A_6 as $L_2(9)$. *Journal of Mathematical Chemistry*, 44(1):5–19, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9288-9.

Fessatidis:2008:ZPE

[1328] Vassilios Fessatidis, Jay D. Mancini, Samuel P. Bowen, and Mauricio Campuzano. Zero point energy of the Pullen–Edmonds Hamiltonian.

Journal of Mathematical Chemistry, 44(1):20–27, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9289-8`.

Oztekin:2008:ERR

[1329] E. Öztekin and S. Özcan. Evaluation of recurrence relationships and numerical solutions for finite rotation matrix elements by using auxiliary functions. *Journal of Mathematical Chemistry*, 44(1):28–45, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9290-2`.

Zhao:2008:FSL

[1330] Xuezhuang Zhao, Zhenfeng Shang, Zucheng Li, Hongwei Sun, Lan Chen, Guichang Wang, Xiufang Xu, Ruifang Li, and Yinming Pan. The fuzzy symmetries for linear tri-atomic $B \cdots A \cdots C$ dynamic systems. *Journal of Mathematical Chemistry*, 44(1):46–74, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9293-z`.

Pulapaka:2008:EAC

[1331] Hari Pulapaka and David R. Gibson. An efficient algorithm for chemical fingerprinting. *Journal of Mathematical Chemistry*, 44(1):75–87, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9294-y`.

Paldus:2008:ASB

[1332] Josef Paldus and Gabriela Thiamová. Approximate symmetry-breaking in the independent particle model of monocyclic completely conjugated polyenes. *Journal of Mathematical Chemistry*, 44(1):88–120, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9295-x`.

Kardos:2008:CEC

[1333] Frantisek Kardos and Riste Skrekovski. Cyclic edge-cuts in fullerene graphs. *Journal of Mathematical Chemistry*, 44(1):121–132, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9296-9`.

Hasanov:2008:AFC

[1334] Alemdar Hasanov and Safak Hasanoglu. Analytical formulaes and comparative analysis for linear models in chronoamperometry under conditions of diffusion and migration. *Journal of Mathematical Chemistry*,

44(1):133–141, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9297-8`.

Sharp:2008:PDM

[1335] Richard Sharp, Abhra Mitra, and Herschel Rabitz. Principles for determining mechanistic pathways from observable quantum control data. *Journal of Mathematical Chemistry*, 44(1):142–171, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9298-7`.

Liu:2008:MSO

[1336] Xingchang Liu, Xiaofan Yang, and Yuan Yan Tang. Molecular solution to the optimal linear arrangement problem based on DNA computation. *Journal of Mathematical Chemistry*, 44(1):172–183, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9299-6`.

Nadarajah:2008:MMF

[1337] Saralees Nadarajah. Models for Mandel's formula. *Journal of Mathematical Chemistry*, 44(1):184–196, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9300-4`.

Guseinov:2008:UTCb

[1338] I. I. Guseinov. Unified treatment of complete orthonormal sets for exponential type vector orbitals of particles with spin 1 in coordinate, momentum and four-dimensional spaces. *Journal of Mathematical Chemistry*, 44(1):197–205, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9301-3`.

Zhang:2008:VDS

[1339] Yusen Zhang and Mingshu Tan. Visualization of DNA sequences based on 3DD-Curves. *Journal of Mathematical Chemistry*, 44(1):206–216, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9302-2`.

Zhang:2008:SCM

[1340] Shuwen Zhang and Dejun Tan. Study of a chemostat model with Beddington–DeAngelis functional response and pulsed input and washout at different times. *Journal of Mathematical Chemistry*, 44

(1):217–227, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9304-0.

Carbo-Dorca:2008:QSM

[1341] Ramon Carbó-Dorca. A quantum similarity matrix (QSM) Aufbau procedure. *Journal of Mathematical Chemistry*, 44(1):228–234, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9305-z.

Zhou:2008:RMT

[1342] Bo Zhou and Nenad Trinajstić. On reciprocal molecular topological index. *Journal of Mathematical Chemistry*, 44(1):235–243, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9306-y.

Craciun:2008:ICR

[1343] Gheorghe Craciun and Casian Pantea. Identifiability of chemical reaction networks. *Journal of Mathematical Chemistry*, 44(1):244–259, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9307-x. See comment [1485].

Roy:2008:ACB

[1344] Amlan K. Roy, Abraham F. Jalbout, and Emil I. Proynov. Accurate calculation of the bound states of Hellmann potential. *Journal of Mathematical Chemistry*, 44(1):260–269, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9308-9.

Zhang:2008:RTP

[1345] Heping Zhang and Dong Ye. k-resonant toroidal polyhexes. *Journal of Mathematical Chemistry*, 44(1):270–285, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9310-2.

Carbo-Dorca:2008:RTD

[1346] Ramon Carbó-Dorca. Riemannian three dimensional molecular spaces. *Journal of Mathematical Chemistry*, 44(1):286–300, July 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9315-x.

Liu:2008:RI

[1347] Huiqing Liu, Mei Lu, and Feng Tian. On the Randić index. *Journal of Mathematical Chemistry*, 44(2):301–310, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-005-9020-6`.

Ayers:2008:CHM

[1348] Paul W. Ayers. Constraints for hierarchies of many electron distribution functions. *Journal of Mathematical Chemistry*, 44(2):311–323, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9261-7`.

Nalewajski:2008:CAC

[1349] R. F. Nalewajski, D. Blazewicz, and J. Mrozek. Compliance approach to coupling between electronic and geometric structures of open and closed molecular systems. *Journal of Mathematical Chemistry*, 44(2):325–364, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9312-0`.

Mamedov:2008:CTC

[1350] B. A. Mamedov and H. Koç. Calculation of two-center overlap integral in molecular coordinate system over Slater type orbital using Löwdin α-radial and Guseinov rotation-angular functions. *Journal of Mathematical Chemistry*, 44(2):365–372, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9313-z`. See corrigendum [1456].

Carbo-Dorca:2008:SFT

[1351] Ramon Carbó-Dorca. Smooth function topological structure descriptors based on graph-spectra. *Journal of Mathematical Chemistry*, 44(2):373–378, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9314-y`.

Arribas:2008:MBS

[1352] E. Arribas, H. Bisswanger, A. Sotos-Lomas, M. Garcia-Moreno, F. Garcia-Canovas, J. Donoso-Pardo, F. Muñoz-Izquierdo, and R. Varon. A method, based on statistical moments, to evaluate the kinetic parameters involved in unstable enzyme systems. *Journal of Mathematical*

Chemistry, 44(2):379–404, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9316-9`.

Chen:2008:RDL

[1353] Haiyan Chen and Fuji Zhang. Resistance distance local rules. *Journal of Mathematical Chemistry*, 44(2):405–417, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9317-8`.

Nalewajski:2008:EBD

[1354] Roman F. Nalewajski. Entropic bond-descriptors of molecular information systems in local resolution. *Journal of Mathematical Chemistry*, 44 (2):419–445, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9318-7`.

Simos:2008:FFS

[1355] T. E. Simos. A family of four-step trigonometrically-fitted methods and its application to the Schrödinger equation. *Journal of Mathematical Chemistry*, 44(2):447–466, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9319-6`.

Pang:2008:ABD

[1356] Guoping Pang and Lansun Chen. Analysis of a Beddington–DeAngelis food chain chemostat with periodically varying substrate. *Journal of Mathematical Chemistry*, 44(2):467–481, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9321-z`.

Simos:2008:CNC

[1357] T. E. Simos. Closed Newton–Cotes trigonometrically-fitted formulae of high order for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 44(2):483–499, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9322-y`.

Zhang:2008:WBC

[1358] Tonghua Zhang, Yu-Chu Tian, and Moses O. Tadé. Wavelet-based collocation method for stiff systems in process engineering. *Journal of Mathematical Chemistry*, 44(2):501–513, August 2008. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9324-9.

Baowan:2008:TMF

[1359] Duangkamon Baowan, Barry J. Cox, and James M. Hill. Toroidal molecules formed from three distinct carbon nanotubes. *Journal of Mathematical Chemistry*, 44(2):515–527, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9325-8.

Velasco:2008:SOD

[1360] R. M. Velasco, F. J. Uribe, and E. Pérez-Chavela. Stratospheric ozone dynamics according to the Chapman mechanism. *Journal of Mathematical Chemistry*, 44(2):529–539, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9326-7.

Duchowicz:2008:POR

[1361] Pablo R. Duchowicz, Martín G. Vitale, and Eduardo A. Castro. Partial order ranking for the aqueous toxicity of aromatic mixtures. *Journal of Mathematical Chemistry*, 44(2):541–549, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9327-6.

Cai:2008:KAN

[1362] Junmeng Cai, Ronghou Liu, and Caixia Huang. Kinetic analysis of non-isothermal solid-state reactions: determination of the kinetic parameters by means of a nonlinear regression method. *Journal of Mathematical Chemistry*, 44(2):551–558, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9328-5.

Hosoya:2008:KSH

[1363] Haruo Hosoya and Ivan Gutman. Kekulé structures of hexagonal chains-some unusual connections. *Journal of Mathematical Chemistry*, 44(2):559–568, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9329-4.

Wang:2008:MRB

[1364] Jun Wang and Yi Zhang. Mathematical relations between codon bias indexes and their applications. *Journal of Mathematical Chemistry*, 44(2):569–575, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9330-y.

Restrepo:2008:DSP

[1365] Guillermo Restrepo and Rainer Brüggemann. Dominance and separability in posets, their application to isoelectronic species with equal total nuclear charge. *Journal of Mathematical Chemistry*, 44(2):577–602, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9331-x.

Guseinov:2008:ACH

[1366] I. I. Guseinov. Application of combined Hartree–Fock–Roothaan theory to molecules with arbitrary number of closed and open shells. *Journal of Mathematical Chemistry*, 44(2):603–609, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9332-9.

Zhou:2008:HI

[1367] Bo Zhou, Xiaochun Cai, and Nenad Trinajstić. On Harary index. *Journal of Mathematical Chemistry*, 44(2):611–618, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-007-9339-2.

Nadarajah:2008:LE

[1368] Saralees Nadarajah. Letter to the Editor. *Journal of Mathematical Chemistry*, 44(2):619–620, August 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-007-9333-8; http://link.springer.com/article/10.1007/s10910-007-9333-8.

Carbo-Dorca:2008:DCR

[1369] Ramon Carbó-Dorca. Diagonal coefficient representation of density functions and quantum similarity measures. *Journal of Mathematical Chemistry*, 44(3):621–627, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9441-0.

Carbo-Dorca:2008:MQS

[1370] Ramon Carbó-Dorca. Molecular quantum similarity measures in Minkowski metric vector semispaces. *Journal of Mathematical Chemistry*, 44(3):628–636, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9442-z.

Sun:2008:DBB

[1371] Mingjing Sun, Yuanshun Tan, and Lansun Chen. Dynamical behaviors of the Brusselator system with impulsive input. *Journal of Mathematical Chemistry*, 44(3):637–649, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9362-y`.

Marrero-Ponce:2008:NTC

[1372] Yovani Marrero-Ponce, Francisco Torrens, Ramón García-Domenech, Sadiel E. Ortega-Broche, and Vicente Romero Zaldivar. Novel 2D TOMOCOMD–CARDD molecular descriptors: atom-based stochastic and non-stochastic bilinear indices and their QSPR applications. *Journal of Mathematical Chemistry*, 44(3):650–673, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9389-0`.

Pang:2008:BCT

[1373] Guoping Pang, Yanlai Liang, and Fengyan Wang. Bifurcation and chaos of Tessiet type food chain chemostat with periodically varying substrate. *Journal of Mathematical Chemistry*, 44(3):674–690, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9347-x`.

Wang:2008:CCB

[1374] Fengyan Wang and Guoping Pang. Competition in a chemostat with Beddington–DeAngelis growth rates and periodic pulsed nutrient. *Journal of Mathematical Chemistry*, 44(3):691–710, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9346-y`.

Dias:2008:IEP

[1375] Jerry Ray Dias. Isomer enumeration of practical benzenoids. *Journal of Mathematical Chemistry*, 44(3):711–724, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9343-6`.

Vukicevic:2008:NOC

[1376] Damir Vukičević and Alexandru T. Balaban. Note on ordering and complexity of Platonic and Archimedean polyhedra based on solid angles. *Journal of Mathematical Chemistry*, 44(3):725–730, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9361-z`.

Hasanov:2008:CAL

[1377] Alemdar Hasanov and Safak Hasanoglu. Comparative analysis of linear and nonlinear models for ion transport problem in chronoamperometry. *Journal of Mathematical Chemistry*, 44(3):731–742, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9350-2`.

Rajamohan:2008:SED

[1378] C. Rajamohan, A. Merwyn Jasper D. Reuben, P. Nithiananthi, and K. Jayakumar. Shape effect of diamagnetic susceptibility of a hydrogenic donor in a nano structured semiconductor systems. *Journal of Mathematical Chemistry*, 44(3):743–748, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9388-1`.

Guseinov:2008:EAF

[1379] I. I. Guseinov and B. A. Mamedov. Evaluation of the auxiliary function G^q_{-ns} using basic overlap integrals over Slater type orbitals. *Journal of Mathematical Chemistry*, 44(3):749–754, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9349-8`.

Marrero-Ponce:2008:CAB

[1380] Yovani Marrero-Ponce, Juan Alberto Castillo-Garit, Eduardo A. Castro, Francisco Torrens, and Richard Rotondo. 3D-chiral (2.5) atom-based TOMOCOMD–CARDD descriptors: theory and QSAR applications to central chirality codification. *Journal of Mathematical Chemistry*, 44 (3):755–786, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9386-3`.

Lo:2008:PMS

[1381] Joseph Q. W. Lo and Bernie D. Shizgal. Pseudospectral methods of solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 44 (3):787–801, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9341-8`.

Nalewajski:2008:IEE

[1382] Roman F. Nalewajski. Internal and external eigenvalue problems of Hermitian operators and their use in electronic structure theory. *Journal*

of Mathematical Chemistry, 44(3):802–815, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9342-7`.

Gubernov:2008:ELN

[1383] V. V. Gubernov, H. S. Sidhu, G. N. Mercer, A. V. Kolobov, and A. A. Polezhaev. The effect of Lewis number variation on combustion waves in a model with chain-branching reaction. *Journal of Mathematical Chemistry*, 44(3):816–830, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9363-x`.

Fu:2008:AKE

[1384] Keang Fu and Xiaorong Yang. Asymptotics of kernel error density estimators in nonlinear autoregressive models. *Journal of Mathematical Chemistry*, 44(3):831–838, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9379-2`.

Guseinov:2008:UTCc

[1385] I. I. Guseinov. Unified treatment of complete orthonormal sets of nonrelativistic, quasirelativistic and relativistic sets of spinor wave functions, and Slater spinor orbitals in coordinate, momentum and four-dimensional spaces. *Journal of Mathematical Chemistry*, 44(3):839–848, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9351-1`.

Rahamathunissa:2008:AHV

[1386] G. Rahamathunissa and L. Rajendran. Application of He's variational iteration method in nonlinear boundary value problems in enzyme–substrate reaction diffusion processes: part 1. The steady-state amperometric response. *Journal of Mathematical Chemistry*, 44(3):849–861, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9340-9`.

Zhu:2008:LCT

[1387] Lemin Zhu. Limit cycles of a three-dimensional bio-reactor with inhibition responses. *Journal of Mathematical Chemistry*, 44(3):862–871, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9387-2`.

Gabarro-Arpa:2008:CPM

[1388] Jacques Gabarro-Arpa. A central partition of molecular conformational space. IV. Extracting information from the graph of cells. *Journal of Mathematical Chemistry*, 44(3):872–883, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9384-5`.

Belkic:2008:UDG

[1389] Dzevad Belkić and Karen Belkić. Unequivocal disentangling genuine from spurious information in time signals: clinical relevance in cancer diagnostics through magnetic resonance spectroscopy. *Journal of Mathematical Chemistry*, 44(3):884–912, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9337-4`.

Karimi:2008:RSC

[1390] Sasan Karimi, Anthony Delgado, and Marty Lewinter. Resonance structure counts in parallelogram-like benzenoids with holes. *Journal of Mathematical Chemistry*, 44(3):913–916, October 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9437-9`.

Mezey:2008:E

[1391] Paul G. Mezey. Editorial. *Journal of Mathematical Chemistry*, 44(4):917, November 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-008-9357-8; http://link.springer.com/article/10.1007/s10910-008-9357-8`.

Brouder:2008:DIG

[1392] Christian Brouder. A differential identity for Green functions. *Journal of Mathematical Chemistry*, 44(4):918–937, November 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9353-z`.

Cassam-Chenai:2008:SAP

[1393] Patrick Cassam-Chenaï and Frédéric Patras. Symmetry-adapted polynomial basis for global potential energy surfaces-applications to XY_4 molecules. *Journal of Mathematical Chemistry*, 44(4):938–966, November 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9354-y`.

Lewin:2008:CES

[1394] Mathieu Lewin. On the computation of excited states with MCSCF methods. *Journal of Mathematical Chemistry*, 44(4):967–980, November 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9355-x`.

Cassam-Chenai:2008:GPH

[1395] Patrick Cassam-Chenaï, Jean-Marc Chiaramello, and Paul G. Mezey. Generalisation of a property of Hamiltonians depending linearly upon a parameter: application to a model of inert gas matrix effect on vibrational spectra. *Journal of Mathematical Chemistry*, 44(4):981–987, November 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9356-9`.

Sutcliffe:2008:WMK

[1396] Brian T. Sutcliffe. What mathematicians know about the solutions of Schrödinger Coulomb Hamiltonian. Should chemists care? *Journal of Mathematical Chemistry*, 44(4):988–1008, November 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9358-7`.

Zhilinskii:2008:REB

[1397] B. I. Zhilinskiĭ. Rearrangement of energy bands: topological aspects. *Journal of Mathematical Chemistry*, 44(4):1009–1022, November 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9359-6`.

Mezey:2008:CCE

[1398] Paul G. Mezey. Charge-conserving electron density averaging for a set of nuclear configurations. *Journal of Mathematical Chemistry*, 44(4):1023–1032, November 2008. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9360-0`.

Mezey:2009:SDP

[1399] Paul G. Mezey. Some dimension problems in molecular databases. *Journal of Mathematical Chemistry*, 45(1):1–6, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9365-8`.

vanRensburg:2009:TLK

[1400] E. J. Janse van Rensburg. Thoughts on lattice knot statistics. *Journal of Mathematical Chemistry*, 45(1):7–38, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9364-9`.

Brak:2009:ESL

[1401] R. Brak, A. L. Owczarek, and A. Rechnitzer. Exact solutions of lattice polymer models. *Journal of Mathematical Chemistry*, 45(1):39–57, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9366-7`.

Zia:2009:PCF

[1402] R. K. P. Zia, Yong Wu, and B. Schmittmann. Percolation of a collection of finite random walks: a model for gas permeation through thin polymeric membranes. *Journal of Mathematical Chemistry*, 45(1):58–64, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9367-6`.

Ord:2009:COR

[1403] G. N. Ord. Counting oriented rectangles and the propagation of waves. *Journal of Mathematical Chemistry*, 45(1):65–71, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9368-5`.

Orlandini:2009:MAP

[1404] E. Orlandini and M. C. Tesi. Modelling the adsorption of a polymer subject to an elongational force by directed walk models. *Journal of Mathematical Chemistry*, 45(1):72–94, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9369-4`.

Oppo:2009:FCT

[1405] Gian-Luca Oppo. Formation and control of Turing patterns and phase fronts in photonics and chemistry. *Journal of Mathematical Chemistry*, 45(1):95–112, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9370-y`.

Owczarek:2009:SAW

[1406] A. L. Owczarek, R. Brak, and A. Rechnitzer. Self-avoiding walks in slits and slabs with interactive walls. *Journal of Mathematical Chemistry*, 45 (1):113–128, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9371-x`.

Simpao:2009:TCAa

[1407] Valentino A. Simpao. Toward chemical applications of Heaviside Operational Ansatz: exact solution of radial Schrödinger equation for nonrelativistic N-particle system with pairwise $\frac{1}{r_{ij}}$ radial potential in quantum phase space. *Journal of Mathematical Chemistry*, 45(1):129–140, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9372-9`. See remarks [2033].

Rohlf:2009:SPS

[1408] Katrin Rohlf. Stochastic phase-space description for reactions that change particle numbers. *Journal of Mathematical Chemistry*, 45(1): 141–160, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9373-8`.

Vazquez:2009:CST

[1409] Uriel Octavio Moreles Vázquez, Wataru Shinoda, Preston B. Moore, Chi cheng Chiu, and Steven O. Nielsen. Calculating the surface tension between a flat solid and a liquid: a theoretical and computer simulation study of three topologically different methods. *Journal of Mathematical Chemistry*, 45(1):161–174, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9374-7`.

Shiokawa:2009:NMD

[1410] K. Shiokawa. Non-Markovian dynamics and entanglement in quantum Brownian motion. *Journal of Mathematical Chemistry*, 45(1): 175–187, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9375-6`.

Venturoli:2009:KPT

[1411] Maddalena Venturoli, Eric Vanden-Eijnden, and Giovanni Ciccotti. Kinetics of phase transitions in two dimensional Ising models studied

with the string method. *Journal of Mathematical Chemistry*, 45(1): 188–222, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9376-5`.

Guttmann:2009:MFI

[1412] Anthony J. Guttmann, Jesper L. Jacobsen, Iwan Jensen, and Sanjay Kumar. Modeling force-induced bio-polymer unfolding. *Journal of Mathematical Chemistry*, 45(1):223–237, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9377-4`.

Alvarez:2009:HOM

[1413] J. Alvarez and C. E. Soteros. Higher order Morita approximations for random copolymer localization. *Journal of Mathematical Chemistry*, 45 (1):238–256, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9378-3`.

Simpao:2009:TCAb

[1414] Valentino A. Simpao. Toward chemical applications of Heaviside Operational Ansatz: exact solution of radial Schrödinger equation for nonrelativistic n-particle system with pairwise $\frac{1}{r_{ij}}$ radial potential in quantum phase space. *Journal of Mathematical Chemistry*, 45(1):257, January 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-008-9400-9; http://link.springer.com/article/10.1007/s10910-008-9400-9`.

Nagy:2009:P

[1415] Csaba L. Nagy and Mircea V. Diudea. Preface. *Journal of Mathematical Chemistry*, 45(2):259–262, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9453-9`.

Brinkmann:2009:NFD

[1416] Gunnar Brinkmann, Jack E. Graver, and Claudia Justus. Numbers of faces in disordered patches. *Journal of Mathematical Chemistry*, 45(2): 263–278, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9403-6`.

Cigher:2009:KSC

[1417] S. Cigher, D. Vukicević, and M. V. Diudea. On Kekulé structures count. *Journal of Mathematical Chemistry*, 45(2):279–286, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9404-5`.

Costescu:2009:QMH

[1418] Adina Costescu, Cristina D. Moldovan, Gabriel Katona, and Mircea V. Diudea. QSAR modeling of human catechol *O*-methyltransferase enzyme kinetics. *Journal of Mathematical Chemistry*, 45(2):287–294, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9405-4`.

Diudea:2009:CP

[1419] Mircea V. Diudea. Cluj polynomials. *Journal of Mathematical Chemistry*, 45(2):295–308, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9406-3`.

Diudea:2009:OPT

[1420] Mircea V. Diudea. Omega polynomial in twisted/chiral polyhex tori. *Journal of Mathematical Chemistry*, 45(2):309–315, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9407-2`.

Diudea:2009:OPU

[1421] M. V. Diudea, S. Cigher, A. E. Vizitiu, M. S. Florescu, and P. E. John. Omega polynomial and its use in nanostructure description. *Journal of Mathematical Chemistry*, 45(2):316–329, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9408-1`.

Diudea:2009:ACF

[1422] Mircea V. Diudea and Aniela E. Vizitiu. Aromaticity of corazulenic fullerenes. *Journal of Mathematical Chemistry*, 45(2):330–353, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9409-0`.

Diudea:2009:RLS

[1423] Mircea V. Diudea. Retro-leapfrog and structure elucidation. *Journal of Mathematical Chemistry*, 45(2):354–363, February 2009. CODEN JM-

CHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9410-7.

Jantschi:2009:SPV

[1424] Lorentz Jäntschi and Mircea V. Diudea. Subgraphs of pair vertices. *Journal of Mathematical Chemistry*, 45(2):364–371, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9411-6.

Kutnar:2009:INP

[1425] Klavdija Kutnar, Urban Borstnik, Dragan Marusic, and Dusanka Janezic. Interconnection networks for parallel molecular dynamics simulation based on Hamiltonian cubic symmetric topology. *Journal of Mathematical Chemistry*, 45(2):372–385, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9412-5.

Lijnen:2009:OAF

[1426] Erwin Lijnen and Arnout Ceulemans. Optimized algorithm to find all symmetry-distinct maps of a graph: application to topology-driven molecular design. *Journal of Mathematical Chemistry*, 45(2):386–405, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9413-4.

Kutnar:2009:DLF

[1427] Klavdija Kutnar, Dragan Marusic, and Damir Vukicević. On decompositions of leapfrog fullerenes. *Journal of Mathematical Chemistry*, 45(2):406–416, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9414-3.

Lijnen:2009:DTM

[1428] E. Lijnen, A. Ceulemans, M. V. Diudea, and Cs. L. Nagy. Double toroids as model systems for carbon nanotube junctions: through-bond currents. *Journal of Mathematical Chemistry*, 45(2):417–430, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9415-2.

Kutnar:2009:AKN

[1429] Klavdija Kutnar, Jelena Sedlar, and Damir Vukicević. On the anti-Kekulé number of leapfrog fullerenes. *Journal of Mathematical Chemistry*, 45(2):431–441, February 2009. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9416-1.

Moldovan:2009:AQS

[1430] Cristina D. Moldovan, Adina Costescu, Gabriel Katona, and Mircea V. Diudea. Application to QSAR studies of 2-furylethylene derivatives. *Journal of Mathematical Chemistry*, 45(2):442–451, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9417-0.

Nagy:2009:ETA

[1431] Csaba L. Nagy, Katalin Nagy, and Mircea V. Diudea. Elongated tori from armchair DWNT. *Journal of Mathematical Chemistry*, 45(2):452–459, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9418-z.

Nakada:2009:TES

[1432] Kyoko Nakada, Kenji Maeda, and Kota Daigoku. Topology and electronic structure of nanotube junctions of tetrapod shape. *Journal of Mathematical Chemistry*, 45(2):460–470, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9419-y.

Peeters:2009:GN

[1433] Adriaan Peeters, Kris Coolsaet, Gunnar Brinkmann, Nicolas Van Cleemput, and Veerle Fack. GrInvIn in a nutshell. *Journal of Mathematical Chemistry*, 45(2):471–477, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9420-5.

Socol:2009:NMF

[1434] Marius Socol and Ioan Bâldea. New method of finding the analytical solutions directly on the base on the reaction mechanism. *Journal of Mathematical Chemistry*, 45(2):478–487, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9421-4.

Xu:2009:HPT

[1435] Shoujun Xu and Heping Zhang. Hosoya polynomials of $TUC_4C_8(S)$ nanotubes. *Journal of Mathematical Chemistry*, 45(2):488–502, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9422-3.

Trobec:2009:CPM

[1436] Roman Trobec, Urban Borstnik, and Dusanka Janezic. Communication performance of d-meshes in molecular dynamics simulation. *Journal of Mathematical Chemistry*, 45(2):503–512, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9423-2`.

Vizitiu:2009:TF

[1437] A. E. Vizitiu, Cs. L. Nagy, M. Stefu, G. Katona, M. V. Diudea, B. Parv, and D. Vukicević. Tubercular fulleroids. *Journal of Mathematical Chemistry*, 45(2):513–524, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9424-1`.

Vukicevic:2009:AFK

[1438] D. Vukicević, S. Cigher, and M. V. Diudea. Analytical formulas for Kekulé structures number in (6,3)VH t [6, n] and (6,3)VH t [8, n] tori. *Journal of Mathematical Chemistry*, 45(2):525–537, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9425-0`.

Vukicevic:2009:PZM

[1439] Damir Vukicević, Sonja Nikolić, and Nenad Trinajstić. On the path-Zagreb matrix. *Journal of Mathematical Chemistry*, 45(2):538–543, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9427-y`.

Mezey:2009:QUM

[1440] Paul G. Mezey. QSAR and the ultimate molecular descriptor: the shape of electron density clouds. *Journal of Mathematical Chemistry*, 45(2):544–549, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9428-x`.

Mezey:2009:ERB

[1441] Paul G. Mezey. Energy relations between small and large unit cell boron-nitrogen polymer analogues of spiral graphite and nanoneedle structures. *Journal of Mathematical Chemistry*, 45(2):550–556, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9429-9`.

Vukicevic:2009:FFC

[1442] Damir Vukicević and Ante Graovac. On functionalized fullerenes $C_{60}X_n$. *Journal of Mathematical Chemistry*, 45(2):557–562, February 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9430-3`.

Belkic:2009:GCS

[1443] Dzevad Belkić and Karen Belkić. The general concept of signal-noise separation (SNS): mathematical aspects and implementation in magnetic resonance spectroscopy. *Journal of Mathematical Chemistry*, 45 (3):563–597, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9344-5`.

Farkas:2009:PFL

[1444] Ödön Farkas, Imre Jákli, Adrián Kalászi, and Gábor Imre. Parameter-free linear relationship (PFLR) and its application to 3D QSAR. *Journal of Mathematical Chemistry*, 45(3):598–606, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9348-9`.

Nalewajski:2009:MSC

[1445] Roman F. Nalewajski. On molecular similarity in communication theory of the chemical bond. *Journal of Mathematical Chemistry*, 45(3): 607–626, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9345-4`.

Zivkovic:2009:ETO

[1446] Tomislav P. Zivković. Exact treatment of open finite-dimensional quantum systems: I. Time-independent case. *Journal of Mathematical Chemistry*, 45(3):627–701, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-007-9336-5`.

Guseinov:2009:UUO

[1447] I. I. Guseinov, B. A. Mamedov, Z. Andic, and S. Cicek. Use of unsymmetrical one-range addition theorems of Slater type orbitals in molecular electronic structure determination. *Journal of Mathematical Chemistry*, 45(3):702–708, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9352-0`.

Nalewajski:2009:CTP

[1448] Roman F. Nalewajski. Communication-theory perspective on valence-bond theory. *Journal of Mathematical Chemistry*, 45(3):709–724, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9385-4`.

Balaban:2009:PP

[1449] Alexandru T. Balaban, Kiran B. Chilakamarri, and Douglas J. Klein. Protochirons and protohelices. *Journal of Mathematical Chemistry*, 45 (3):725–747, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9382-7`.

Lin:2009:EKE

[1450] Chun-Chi Lin and Hartmut R. Schwetlick. Evolving a Kirchhoff elastic rod without self-intersections. *Journal of Mathematical Chemistry*, 45 (3):748–768, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9383-6`.

Capela:2009:RAA

[1451] Jorge M. V. Capela, Marisa V. Capela, and Clóvis A. Ribeiro. Rational approximations of the Arrhenius integral using Jacobi fractions and Gaussian quadrature. *Journal of Mathematical Chemistry*, 45(3): 769–775, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9381-8`.

Nalewajski:2009:MPE

[1452] Roman F. Nalewajski. Manifestations of Pauli exclusion principle in communication-theory of the chemical bond. *Journal of Mathematical Chemistry*, 45(3):776–789, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9380-9`.

Belkic:2009:EQT

[1453] Dzevad Belkić and Karen Belkić. Exact quantification of time signals from magnetic resonance spectroscopy by the fast Padé transform with applications to breast cancer diagnostics. *Journal of Mathematical Chemistry*, 45(3):790–818, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9462-8`.

Belkic:2009:URM

[1454] Dzevad Belkić and Karen Belkić. Unequivocal resolution of multiplets in MR spectra for prostate cancer diagnostics achieved by the fast Padé transform. *Journal of Mathematical Chemistry*, 45(3):819–858, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9484-2`.

Plakhutin:2009:CCO

[1455] Boris N. Plakhutin and Ernest R. Davidson. Comment on "Combined open shell Hartree–Fock theory of atomic-molecular and nuclear systems" [J. Math. Chem. **42** (2007) 177]. *Journal of Mathematical Chemistry*, 45 (3):859–866, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9396-1`. See [1151].

Mamedov:2009:CTCa

[1456] B. A. Mamedov and H. Koç. Calculation of two-center overlap integral in molecular coordinate system over Slater type orbital using Löwdin α-radial and Guseinov rotation-angular functions [vol 44, pg 365, 2008]. *Journal of Mathematical Chemistry*, 45(3):867, March 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9449-5; http://link.springer.com/content/pdf/10.1007/s10910-008-9449-5.pdf`. See [1350].

Batagiannis:2009:UBPa

[1457] Athanasios Batagiannis, Thomas Wüst, and Jürg Hulliger. Universality behaviour for polarity formation in channel-type inclusion compounds. *Journal of Mathematical Chemistry*, 45(4):869–881, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9433-0`.

Batagiannis:2009:UBPb

[1458] Athanasios Batagiannis, Thomas Wüst, and Jürg Hulliger. Universality behaviour for polarity formation in channel-type inclusion compounds. *Journal of Mathematical Chemistry*, 45(4):882–883, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9469-1; http://link.springer.com/content/pdf/10.1007/s10910-008-9469-1.pdf`.

Pashaev:2009:UFSa

[1459] F. G. Pashaev. Use of filter–Steinborn B and Guseinov Q^q_{ns} auxiliary functions in evaluation of two-center overlap integrals over Slater type orbitals. *Journal of Mathematical Chemistry*, 45(4):884–890, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9436-x`.

Pashaev:2009:UFSb

[1460] F. G. Pashaev. Use of filter–Steinborn B and Guseinov Q^q_{ns} auxiliary functions in evaluation of two-center overlap integrals over Slater type orbitals. *Journal of Mathematical Chemistry*, 45(4):891, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9488-y; http://link.springer.com/content/pdf/10.1007/s10910-008-9488-y.pdf`.

Klein:2009:PIMa

[1461] D. J. Klein, A. Ryhzov, and V. Rosenfeld. Permutational isomers on a molecular skeleton with neighbor-excluding ligands. *Journal of Mathematical Chemistry*, 45(4):892–909, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9461-9`.

Klein:2009:PIMb

[1462] D. J. Klein, A. Ryzhov, and V. Rosenfeld. Permutational isomers on a molecular skeleton with neighbor-excluding ligands. *Journal of Mathematical Chemistry*, 45(4):910, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9503-3; http://link.springer.com/content/pdf/10.1007/s10910-008-9503-3.pdf`.

Martinez:2009:RFS

[1463] Jorge Martínez and Alejandro Toro-Labbé. The reaction force. A scalar property to characterize reaction mechanisms. *Journal of Mathematical Chemistry*, 45(4):911–927, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9478-0`. See minor erratum [1464] about figure label.

Martinez:2009:ERF

[1464] Jorge Martínez and Alejandro Toro-Labbé. Erratum: The reaction force. A scalar property to characterize reaction mecha-

nisms. *Journal of Mathematical Chemistry*, 45(4):928–929, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9521-9; http://link.springer.com/content/pdf/10.1007/s10910-009-9521-9.pdf`. See [1463].

Livadiotis:2009:ATSa

[1465] George Livadiotis. Approach on Tsallis statistical interpretation of hydrogen-atom by adopting the generalized radial distribution function. *Journal of Mathematical Chemistry*, 45(4):930–939, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9524-6`.

Livadiotis:2009:ATSb

[1466] George Livadiotis. Approach on Tsallis statistical interpretation of hydrogen-atom by adopting the generalized radial distribution function. *Journal of Mathematical Chemistry*, 45(4):940, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9537-1; http://link.springer.com/content/pdf/10.1007/s10910-009-9537-1.pdf`.

Alpar-Vajk:2009:BRD

[1467] Kramer Alpar-Vajk. A bound for the reversal distance of genome rearrangements. *Journal of Mathematical Chemistry*, 45(4):941–945, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9444-x`.

Guseinov:2009:TCO

[1468] I. I. Guseinov. Theory of complete orthonormal relativistic vector wave function sets and Slater type relativistic vector orbitals in coordinate, momentum and four-dimensional spaces. *Journal of Mathematical Chemistry*, 45(4):946–952, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9434-z`.

Lim:2009:CIA

[1469] Teik-Cheng Lim. Coefficient interrelatedness among polynomial potential functions of diatomic molecules. *Journal of Mathematical Chemistry*, 45 (4):953–961, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9440-1`.

Li:2009:MET

[1470] Xueliang Li, Xiangmei Yao, Jianbin Zhang, and Ivan Gutman. Maximum energy trees with two maximum degree vertices. *Journal of Mathematical Chemistry*, 45(4):962–973, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9394-3`.

Guseinov:2009:UAF

[1471] I. I. Guseinov. Use of auxiliary functions Q^q_{ns} and G^q_{-ns} in evaluation of multicenter integrals over integer and noninteger n-Slater type orbitals arising in Hartree–Fock–Roothaan equations for molecules. *Journal of Mathematical Chemistry*, 45(4):974–980, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9431-2`.

Dey:2009:CCR

[1472] Bijoy K. Dey and Paul W. Ayers. Computing the chemical reaction path with a ray-based fast marching technique for solving the Hamilton–Jacobi equation in a general coordinate system. *Journal of Mathematical Chemistry*, 45(4):981–1003, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9395-2`.

Smolenskii:2009:RMT

[1473] E. A. Smolenskii, E. V. Shuvalova, L. K. Maslova, I. V. Chuvaeva, and M. S. Molchanova. Reduced matrix of topological distances with a minimum number of independent parameters: distance vectors and molecular codes. *Journal of Mathematical Chemistry*, 45(4):1004–1020, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9393-4`.

Kral:2009:LCF

[1474] Daniel Král', Ondrej Pangrác, Jean-Sébastien Sereni, and Riste Skrekovski. Long cycles in fullerene graphs. *Journal of Mathematical Chemistry*, 45(4):1021–1031, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9390-7`.

Guseinov:2009:UTN

[1475] I. I. Guseinov. Unified treatment of nonrelativistic and quasirelativistic atomic integrals over complete orthonormal sets of Ψ^α-exponential type orbitals. *Journal of Mathematical Chemistry*, 45(4):1032–1040, April

2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9432-1; http://link.springer.com/content/pdf/10.1007/s10910-008-9432-1.pdf.

Nalewajski:2009:EDC

[1476] Roman F. Nalewajski. Entropic descriptors of the chemical bond in H_2: local resolution of Stockholder atoms. *Journal of Mathematical Chemistry*, 45(4):1041–1054, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9391-6.

Inostroza:2009:VSC

[1477] Natalia Inostroza, Ricardo Letelier, and María Luisa Senent. On the variational solution of the coupled breathing rotation-vibration of a spherical top molecule. *Journal of Mathematical Chemistry*, 45(4):1055–1059, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9392-5.

Zivkovic:2009:VIE

[1478] Tomislav P. Zivković. Vibrational isotope effect by the low rank perturbation method. *Journal of Mathematical Chemistry*, 45(4):1060–1101, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9445-9.

Anastassi:2009:FTS

[1479] Z. A. Anastassi and T. E. Simos. A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. *Journal of Mathematical Chemistry*, 45 (4):1102–1129, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9439-7.

Doslic:2009:FMP

[1480] Tomislav Doslić. Finding more perfect matchings in leapfrog fullerenes. *Journal of Mathematical Chemistry*, 45(4):1130–1136, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9435-y.

Ikhdair:2009:EQR

[1481] Sameer M. Ikhdair and Ramazan Sever. Exact quantization rule to the Kratzer-type potentials: an application to the diatomic molecules. *Jour-*

nal of Mathematical Chemistry, 45(4):1137–1152, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9438-8`.

Ozcan:2009:AET

[1482] Selda Özcan and Emin Öztekin. Analytical evaluation for two-center nuclear attraction integrals over Slater type orbitals by using Fourier transform method. *Journal of Mathematical Chemistry*, 45(4):1153–1165, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9398-z`. See comment [1483].

Guseinov:2009:CAE

[1483] I. I. Guseinov. Comment on "Analytical evaluation for two-center nuclear attraction integrals over Slater type orbitals by using Fourier transform method" by S. Özcan and E. Öztekin (J. Math. Chem. DOI 10.1007/s10910-008-9398-z). *Journal of Mathematical Chemistry*, 45(4): 1166–1169, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9481-5`. See [1482].

Nadarajah:2009:LE

[1484] Saralees Nadarajah. Letter to the Editor. *Journal of Mathematical Chemistry*, 45(4):1170–1171, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-008-9443-y; http://link.springer.com/article/10.1007/s10910-008-9443-y`.

Szederkenyi:2009:CIC

[1485] Gábor Szederkényi. Comment on "Identifiability of chemical reaction networks" by G. Craciun and C. Pantea. *Journal of Mathematical Chemistry*, 45(4):1172–1174, April 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9499-8`. See [1343].

Angyan:2009:WRN

[1486] János G. Ángyán. Wigner's $(2n+1)$ rule for nonlinear Schrödinger equations. *Journal of Mathematical Chemistry*, 46(1):1–14, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9497-x`.

Pogliani:2009:GT

[1487] Lionello Pogliani. Graphs and thermodynamics. *Journal of Mathematical Chemistry*, 46(1):15–23, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9452-x`.

Ruiz:2009:EHCa

[1488] María Belén Ruiz. Evaluation of Hylleraas–CI atomic integrals by integration over the coordinates of one electron. I. Three-electron integrals. *Journal of Mathematical Chemistry*, 46(1):24–64, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9397-0`.

Yuan:2009:LSR

[1489] Xi-Ying Yuan, Jia-Yu Shao, and Chang-Xiang He. On the Laplacian spectral radii of trees with perfect matchings. *Journal of Mathematical Chemistry*, 46(1):65–85, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9399-y`.

Ayers:2009:PLB

[1490] Paul W. Ayers. A perspective on the link between the exchange(-correlation) hole and dispersion forces. *Journal of Mathematical Chemistry*, 46(1):86–96, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9451-y`.

Romanowski:2009:TCO

[1491] Zbigniew Romanowski and Abraham F. Jalbout. Two-center overlap integrals, three dimensional adaptive integration, and prolate ellipsoidal coordinates. *Journal of Mathematical Chemistry*, 46(1):97–107, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9401-8`.

Aihara:2009:ADP

[1492] Jun ichi Aihara and Masakazu Makino. Aromaticity and diatropicity of p-polyphenyl-α, ω-quinododimethides. *Journal of Mathematical Chemistry*, 46(1):108–116, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9402-7`.

Bucknum:2009:CTC

[1493] Michael J. Bucknum and Eduardo A. Castro. Chemical topology of crystalline matter and the transcendental numbers φ, e, and π. *Journal of Mathematical Chemistry*, 46(1):117–138, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9446-8`.

Berkdemir:2009:NAD

[1494] Cüneyt Berkdemir. A novel angle-dependent potential and its exact solution. *Journal of Mathematical Chemistry*, 46(1):139–154, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9447-7`.

Suarez:2009:TCD

[1495] Jesús Suárez, Enrique Gancedo, José Manuel Álvarez, and Antonio Morán. Truncating and chamfering diagrams of regular polyhedra. *Journal of Mathematical Chemistry*, 46(1):155–163, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9448-6`.

Avery:2009:ACI

[1496] James Avery and John Avery. Atomic core-ionization energies; approximately piecewise-linear and linear relationships. *Journal of Mathematical Chemistry*, 46(1):164–181, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9450-z`.

Kang:2009:NCO

[1497] Ling Kang, Honglin Li, Xiaoyu Zhao, Hualiang Jiang, and Xicheng Wang. A novel conformation optimization model and algorithm for structure-based drug design. *Journal of Mathematical Chemistry*, 46(1):182–198, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9454-8`.

Huang:2009:BSM

[1498] Xuncheng Huang and Lemin Zhu. Bifurcation in the stable manifold of the bioreactor with nth and mth order polynomial yields. *Journal of Mathematical Chemistry*, 46(1):199–213, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9455-7`.

Heuberger:2009:CTM

[1499] Clemens Heuberger and Stephan G. Wagner. Chemical trees minimizing energy and Hosoya index. *Journal of Mathematical Chemistry*, 46 (1):214–230, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9456-6`.

Szmytkowski:2009:DAL

[1500] Radosław Szmytkowski. On the derivative of the associated Legendre function of the first kind of integer degree with respect to its order (with applications to the construction of the associated Legendre function of the second kind of integer degree and order). *Journal of Mathematical Chemistry*, 46(1):231–260, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9457-5`.

Pipek:2009:KEO

[1501] János Pipek and Szilvia Nagy. The kinetic energy operator in the subspaces of wavelet analysis. *Journal of Mathematical Chemistry*, 46 (1):261–282, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9458-4`.

Zhou:2009:RDK

[1502] Bo Zhou and Nenad Trinajstić. On resistance-distance and Kirchhoff index. *Journal of Mathematical Chemistry*, 46(1):283–289, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9459-3`.

Li:2009:NAM

[1503] Banghe Li, Bo Li, and Yuefeng Shen. A novel approach to measure all rate constants in the simplest enzyme kinetics model. *Journal of Mathematical Chemistry*, 46(1):290–301, June 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9460-x`.

Nelson:2009:ACM

[1504] M. I. Nelson and H. S. Sidhu. Analysis of a chemostat model with variable yield coefficient: Tessier kinetics. *Journal of Mathematical Chemistry*, 46 (2):303–321, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9463-7`.

Donnell:2009:SGM

[1505] Pete Donnell, Murad Banaji, and Stephen Baigent. Stability in generic mitochondrial models. *Journal of Mathematical Chemistry*, 46(2):322–339, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9464-6`.

Li:2009:SRG

[1506] J. Li, W. C. Shiu, W. H. Chan, and A. Chang. On the spectral radius of graphs with connectivity at most k. *Journal of Mathematical Chemistry*, 46(2):340–346, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9465-5`.

Guo:2009:ZZP

[1507] Qiuzhi Guo, Hanyuan Deng, and Dandan Chen. Zhang–Zhang polynomials of cyclo-polyphenacenes. *Journal of Mathematical Chemistry*, 46 (2):347–362, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9466-4`. See comment [1978].

Baeurle:2009:MMP

[1508] S. A. Baeurle. Multiscale modeling of polymer materials using field-theoretic methodologies: a survey about recent developments. *Journal of Mathematical Chemistry*, 46(2):363–426, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9467-3`.

Ivanauskas:2009:CMY

[1509] Feliksas Ivanauskas, Aivaras Kareiva, and Bogdan Lapcun. Computational modelling of the YAG synthesis. *Journal of Mathematical Chemistry*, 46(2):427–442, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9468-2`.

Kardos:2009:FGE

[1510] Frantisek Kardos, Daniel Král', Jozef Miskuf, and Jean-Sébastien Sereni. Fullerene graphs have exponentially many perfect matchings. *Journal of Mathematical Chemistry*, 46(2):443–447, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9471-7`.

Oztekin:2009:ANT

[1511] Emin Öztekin. Analytical and numerical treatment of auxiliary function $B_{m'm}{}^{j}(\beta)$ for finite rotation matrix elements. *Journal of Mathematical Chemistry*, 46(2):448–458, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9470-8`.

Rehim:2009:MAN

[1512] Mehbuba Rehim and Zhidong Teng. Mathematical analysis on nonautonomous Droop model for phytoplankton growth in a chemostat: boundedness, permanence and extinction. *Journal of Mathematical Chemistry*, 46(2):459–483, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9472-6`.

Menadakis:2009:IMS

[1513] M. Menadakis, G. Maroulis, and P. G. Koutsoukos. Incorporation of Mg^{2+}, Sr^{2+}, Ba^{2+} and Zn^{2+} into aragonite and comparison with calcite. *Journal of Mathematical Chemistry*, 46(2):484–491, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9490-4`.

Berkdemir:2009:RVE

[1514] Cüneyt Berkdemir. Ro-vibrating energy states of a diatomic molecule in an empirical potential. *Journal of Mathematical Chemistry*, 46(2):492–501, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9473-5`.

Jiao:2009:DAC

[1515] Jianjun Jiao and Lansun Chen. Dynamical analysis of a chemostat model with delayed response in growth and pulse input in polluted environment. *Journal of Mathematical Chemistry*, 46(2):502–513, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9474-4`.

Das:2009:NUB

[1516] Kinkar Ch. Das, Ivan Gutman, and Bo Zhou. New upper bounds on Zagreb indices. *Journal of Mathematical Chemistry*, 46(2):514–521, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9475-3`.

Gutman:2009:TWI

[1517] Ivan Gutman, Boris Furtula, and Miroslav Petrović. Terminal Wiener index. *Journal of Mathematical Chemistry*, 46(2):522–531, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9476-2`.

March:2009:ESO

[1518] N. H. March and G. G. N. Angilella. Electronic states in ordered and disordered quantum networks: with applications to graphene and to boron nanotubes. *Journal of Mathematical Chemistry*, 46(2):532–549, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9477-1`.

Rajendran:2009:TWS

[1519] L. Rajendran and R. Senthamarai. Traveling-wave solution of non-linear coupled reaction diffusion equation arising in mathematical chemistry. *Journal of Mathematical Chemistry*, 46(2):550–561, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9479-z`.

Zhang:2009:FAP

[1520] Shengli Zhang and Tianming Wang. Feature analysis of protein structure by using discrete Fourier transform and continuous wavelet transform. *Journal of Mathematical Chemistry*, 46(2):562–568, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9480-6`.

Lim:2009:ADR

[1521] Teik-Cheng Lim. Approximation of the Dymond–Rigby–Smith potential function using the Lennard-Jones form. *Journal of Mathematical Chemistry*, 46(2):569–575, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9482-4`.

Zhang:2009:EET

[1522] Dongfang Zhang. Exploration for electronic transitions and photodissociation mechanism of hydrogen iodide. *Journal of Mathematical Chemistry*, 46(2):576–585, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9483-3`.

Arimoto:2009:NRS

[1523] Shigeru Arimoto. Normed repeat space and its super spaces: fundamental notions for the second generation Fukui project. *Journal of Mathematical Chemistry*, 46(2):586–591, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9486-0`.

Hu:2009:APP

[1524] Guang Hu, Xin-Dong Zhai, Dan Lu, and Wen-Yuan Qiu. The architecture of platonic polyhedral links. *Journal of Mathematical Chemistry*, 46 (2):592–603, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9487-z`.

Panopoulos:2009:TOS

[1525] G. A. Panopoulos, Z. A. Anastassi, and T. E. Simos. Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions. *Journal of Mathematical Chemistry*, 46(2):604–620, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9506-0`.

Anastassi:2009:NMD

[1526] Z. A. Anastassi, D. S. Vlachos, and T. E. Simos. A new methodology for the development of numerical methods for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 46 (2):621–651, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9507-z`.

Anastassi:2009:NMC

[1527] Z. A. Anastassi, D. S. Vlachos, and T. E. Simos. A new methodology for the construction of numerical methods for the approximate solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 46 (2):652–691, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9508-y`.

Vlachos:2009:HOM

[1528] D. S. Vlachos, Z. A. Anastassi, and T. E. Simos. High order multistep methods with improved phase-lag characteristics for the integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 46(2): 692–725, August 2009. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9509-x.

Simos:2009:P

[1529] T. E. Simos, A. D. Zdetsis, G. Psihoyios, and Zacharias Anastassi. Preface. *Journal of Mathematical Chemistry*, 46(3):727–728, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-009-9563-z; http://link.springer.com/article/10.1007/s10910-009-9563-z.

Duce:2009:RNN

[1530] Celia Duce, Alessio Micheli, Roberto Solaro, Antonina Starita, and Maria Rosaria Tiné. Recursive neural networks prediction of glass transition temperature from monomer structure: an application to acrylic and methacrylic polymers. *Journal of Mathematical Chemistry*, 46(3):729–755, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9547-z.

Kvamme:2009:MES

[1531] Bjørn Kvamme, Tatyana Kuznetsova, and Daniel Uppstad. Modelling excess surface energy in dry and wetted calcite systems. *Journal of Mathematical Chemistry*, 46(3):756–762, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9548-y.

Svandal:2009:MDC

[1532] A. Svandal and B. Kvamme. Modeling the dissociation of carbon dioxide and methane hydrate using the phase field theory. *Journal of Mathematical Chemistry*, 46(3):763–769, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9545-1.

Dorao:2009:TPL

[1533] C. A. Dorao and H. A. Jakobsen. Time-property least-squares spectral method for population balance equations. *Journal of Mathematical Chemistry*, 46(3):770–780, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9546-0.

Takahashi:2009:HER

[1534] Hideaki Takahashi, Fumihiro Miki, Hajime Ohno, Ryohei Kishi, Suguru Ohta, Shin ichi Furukawa, and Masayoshi Nakano. Hydration effects on

the reaction with an open-shell transition state: QM/MM-ER study for the dehydration reaction of alcohol in hot water. *Journal of Mathematical Chemistry*, 46(3):781–794, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9544-2`.

Porras:2009:TAA

[1535] I. Porras. Tests and applications for atoms of an optimized semiexplicit density functional method. *Journal of Mathematical Chemistry*, 46(3): 795–810, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9554-0`.

Buanes:2009:TAM

[1536] Trygve Buanes, Bjørn Kvamme, and Atle Svandal. Two approaches for modelling hydrate growth. *Journal of Mathematical Chemistry*, 46(3): 811–819, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9551-3`.

Rastija:2009:MMW

[1537] V. Rastija, S. Nikolić, and M. Medić-Sarić. Molecular modeling of wine polyphenols. *Journal of Mathematical Chemistry*, 46(3):820–833, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9552-2`.

Meral:2009:DEF

[1538] Esma Meral and Metin Demiralp. Determination of the external field amplitude and deviation parameter through expectation value based quantum optimal control of multiharmonic oscillators under linear control agents. *Journal of Mathematical Chemistry*, 46(3):834–852, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9550-4`.

Urbano-Cuadrado:2009:NQS

[1539] Manuel Urbano-Cuadrado, Irene Luque Ruiz, and Miguel Ángel Gómez-Nieto. A new quantitative structure-property relationship approach using dissimilarity measurements based on topological distances of non-isomorphic subgraphs. *Journal of Mathematical Chemistry*, 46(3):853–865, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9562-0`.

Psihoyios:2009:FNM

[1540] G. Psihoyios. A family of numerical multistep methods with three distinct schemes: explicit advanced step-point (EAS) methods and the EAS1 approach. *Journal of Mathematical Chemistry*, 46(3):866–895, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9561-1`.

Tsitouras:2009:SDR

[1541] Ch. Tsitouras and I. Th. Famelis. Symbolic derivation of Runge–Kutta–Nyström order conditions. *Journal of Mathematical Chemistry*, 46(3): 896–912, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9560-2`.

Zenkevich:2009:APC

[1542] Igor G. Zenkevich. Approximation of any physicochemical constants of homologues with the use of recurrect functions. *Journal of Mathematical Chemistry*, 46(3):913–933, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9559-8`.

Garoufalis:2009:OGE

[1543] C. S. Garoufalis. Optical gap and excitation energies of small Ge nanocrystals. *Journal of Mathematical Chemistry*, 46(3):934–941, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9558-9`.

Zdetsis:2009:MSG

[1544] A. D. Zdetsis, C. S. Garoufalis, and E. N. Koukaras. Mixed silicon-germanium nanocrystals: a detailed study of Si_xGe_{47-x}:H. *Journal of Mathematical Chemistry*, 46(3):942–951, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9555-z`.

Garoufalis:2009:OPU

[1545] C. S. Garoufalis and A. D. Zdetsis. Optical properties of ultra small Si nanoparticles: potential role of surface reconstruction and oxygen contamination. *Journal of Mathematical Chemistry*, 46(3):952–961, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9556-y`.

Bacalis:2009:PHT

[1546] N. C. Bacalis and A. D. Zdetsis. Properties of hydrogen terminated silicon nanocrystals via a transferable tight-binding Hamiltonian, based on ab-initio results. *Journal of Mathematical Chemistry*, 46(3):962–970, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9557-x`.

Zdetsis:2009:PSN

[1547] A. D. Zdetsis, E. N. Koukaras, and C. S. Garoufalis. A parallel study of Ni@Si_{12} and Cu@Si_{12} nanoclusters. *Journal of Mathematical Chemistry*, 46(3):971–980, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9549-x`.

Simos:2009:NNT

[1548] T. E. Simos. A new Numerov-type method for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 46(3): 981–1007, October 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9553-1`.

Vlachos:2009:HOP

[1549] D. S. Vlachos, Z. A. Anastassi, and T. E. Simos. High order phase fitted multistep integrators for the Schrödinger equation with improved frequency tolerance. *Journal of Mathematical Chemistry*, 46(4):1009–1049, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9510-4`.

Zhang:2009:MOS

[1550] Haitao Zhang, Yuan Zhou, Ping Cheng, Sunhua Deng, Xuejun Cui, and Hongyan Wang. Multi-objective simultaneous prediction of waterborne coating properties. *Journal of Mathematical Chemistry*, 46(4): 1050–1059, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9489-x`.

Toropov:2009:QMO

[1551] A. A. Toropov, A. P. Toropova, and E. Benfenati. QSPR modeling of octanol water partition coefficient of platinum complexes by InChI-based optimal descriptors. *Journal of Mathematical Chemistry*, 46(4): 1060–1073, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9491-3.

Guo:2009:PST

[1552] Hongjian Guo and Lansun Chen. Periodic solution of a turbidostat system with impulsive state feedback control. *Journal of Mathematical Chemistry*, 46(4):1074–1086, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9492-2.

Kozlowski:2009:DRR

[1553] M. Kozlowski and R. Ralowski. The dielectric response with respect to the weight distribution of relaxation times. *Journal of Mathematical Chemistry*, 46(4):1087–1102, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9493-1.

Erman:2009:LCF

[1554] Rok Erman, Frantisek Kardos, and Jozef Miskuf. Long cycles in fullerene graphs. *Journal of Mathematical Chemistry*, 46(4):1103–1111, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9495-z.

Brinkmann:2009:GWC

[1555] Gunnar Brinkmann. Generating water clusters and other directed graphs. *Journal of Mathematical Chemistry*, 46(4):1112–1121, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9496-y.

Berkdemir:2009:MSD

[1556] Cüneyt Berkdemir and Ramazan Sever. Modified l-states of diatomic molecules subject to central potentials plus an angle-dependent potential. *Journal of Mathematical Chemistry*, 46(4):1122–1136, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9498-9.

Zheng:2009:PIB

[1557] Xiaoqi Zheng, Yongchao Dou, and Jun Wang. Phylogenetic inference from binary sequences reduced by primary DNA sequences. *Journal of Mathematical Chemistry*, 46(4):1137–1148, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9504-2.

Zheng:2009:CBM

[1558] Xiaoqi Zheng, Chun Li, and Jun Wang. A complexity-based measure and its application to phylogenetic analysis. *Journal of Mathematical Chemistry*, 46(4):1149–1157, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9511-3`.

Anastassi:2009:FRK

[1559] Z. A. Anastassi, D. S. Vlachos, and T. E. Simos. A family of Runge–Kutta methods with zero phase-lag and derivatives for the numerical solution of the Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 46(4):1158–1171, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9505-1`.

Zhou:2009:ECI

[1560] Bo Zhou and Nenad Trinajstić. On extended connectivity indices. *Journal of Mathematical Chemistry*, 46(4):1172–1180, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9500-6`.

Rech:2009:PFH

[1561] Mathias Rech, Athanasios Batagiannis, and Jürg Hulliger. Polarity formation by a higher order interaction Markov-like chain. *Journal of Mathematical Chemistry*, 46(4):1181–1187, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9501-5`.

Hasanov:2009:ANI

[1562] Alemdar Hasanov, Burhan Pektas, and Safak Hasanoglu. An analysis of nonlinear ion transport model including diffusion and migration. *Journal of Mathematical Chemistry*, 46(4):1188–1202, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9502-4`.

Zhang:2009:NLZ

[1563] Yi Zhang, Junkang Hao, Changjie Zhou, and Kai Chang. Normalized Lempel–Ziv complexity and its application in bio-sequence analysis. *Journal of Mathematical Chemistry*, 46(4):1203–1212, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9512-2`.

Liu:2009:PPE

[1564] Zhijun Liu, Jing Hui, and Jianhua Wu. Permanence and partial extinction in an impulsive delay competitive system with the effect of toxic substances. *Journal of Mathematical Chemistry*, 46(4):1213–1231, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9513-1`.

Toropov:2009:AIB

[1565] Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Danuta Leszczynska, and Jerzy Leszczynski. Additive InChI-based optimal descriptors: QSPR modeling of fullerene C_{60} solubility in organic solvents. *Journal of Mathematical Chemistry*, 46(4):1232–1251, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9514-0`.

Zhou:2009:NCI

[1566] Bo Zhou and Nenad Trinajstić. On a novel connectivity index. *Journal of Mathematical Chemistry*, 46(4):1252–1270, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9515-z`.

Chan:2009:MNO

[1567] Yue Chan, Ngamta Thamwattana, Grant M. Cox, and James M. Hill. Mechanics of nanoscale orbiting systems. *Journal of Mathematical Chemistry*, 46(4):1271–1291, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9516-y`.

Lee:2009:RMM

[1568] Chang Hyeong Lee and Roger Lui. A reduction method for multiple time scale stochastic reaction networks. *Journal of Mathematical Chemistry*, 46(4):1292–1321, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9517-x`.

Ruiz:2009:EHCb

[1569] María Belén Ruiz. Evaluation of Hylleraas–CI atomic integrals by integration over the coordinates of one electron. II. Four-electron integrals. *Journal of Mathematical Chemistry*, 46(4):1322–1355, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-008-9518-9`.

Mikulski:2009:SQM

[1570] Damian Mikulski, Marcin Molski, and Jerzy Konarski. Supersymmetry quantum mechanics and the asymptotic iteration method. *Journal of Mathematical Chemistry*, 46(4):1356–1368, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9519-3`.

Vukicevic:2009:TIB

[1571] Damir Vukicević and Boris Furtula. Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *Journal of Mathematical Chemistry*, 46(4):1369–1376, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9520-x`.

Das:2009:BHI

[1572] Kinkar Ch. Das, Bo Zhou, and N. Trinajstić. Bounds on Harary index. *Journal of Mathematical Chemistry*, 46(4):1377–1393, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9522-8`.

Tang:2009:BAR

[1573] Yanbin Tang and Jianli Wang. Bifurcation analysis on a reactor model with combination of quadratic and cubic steps. *Journal of Mathematical Chemistry*, 46(4):1394–1408, November 2009. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9523-7`.

Liu:2010:SRE

[1574] Ying Liu. Some results on energy of unicyclic graphs with n vertices. *Journal of Mathematical Chemistry*, 47(1):1–10, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9528-2`.

Lv:2010:OTG

[1575] Xuezheng Lv, Yan Yan, Aimei Yu, and Jingjing Zhang. Ordering trees with given pendent vertices with respect to Merrifield–Simmons indices and Hosoya indices. *Journal of Mathematical Chemistry*, 47(1):11–20, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9526-4`.

Das:2010:MER

[1576] Kinkar Ch. Das. Maximum eigenvalue of the reciprocal distance matrix. *Journal of Mathematical Chemistry*, 47(1):21–28, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9529-1`.

Zhang:2010:SEN

[1577] Dongfang Zhang. Studies on the effects of nonadiabatic behavior during the course of HBr photolysis. *Journal of Mathematical Chemistry*, 47 (1):29–40, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9527-3`.

Bielinska-Waz:2010:FCS

[1578] Dorota Bielińska-Waz. Four-component spectral representation of DNA sequences. *Journal of Mathematical Chemistry*, 47(1):41–51, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9535-3`.

Iliev:2010:MCG

[1579] Valentin Vankov Iliev. A mathematical characterization of the groups of substitution isomerism of the linear alkanes. *Journal of Mathematical Chemistry*, 47(1):52–61, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9534-4`.

Li:2010:EAO

[1580] Xianyue Li and Heping Zhang. Embedding on alphabet overlap digraphs. *Journal of Mathematical Chemistry*, 47(1):62–71, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9530-8`.

Mansour:2010:WHW

[1581] Toufik Mansour and Matthias Schork. Wiener, hyper-Wiener, detour and hyper-detour indices of bridge and chain graphs. *Journal of Mathematical Chemistry*, 47(1):72–98, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9531-7`.

Demiralp:2010:NFA

[1582] Metin Demiralp. No fluctuation approximation in any desired precision for univariate function matrix representations. *Journal of Mathematical*

Chemistry, 47(1):99–110, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9533-5`.

Shuping:2010:SAS

[1583] Li Shuping, Pei Yongzhen, Li Changguo, and Gao Shujing. Stability analysis for a single-species chemostat model with age structure and contribution of population to resource. *Journal of Mathematical Chemistry*, 47 (1):111–122, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9532-6`.

Meng:2010:DAM

[1584] Xinzhu Meng, Zhenqing Li, and Juan J. Nieto. Dynamic analysis of Michaelis–Menten chemostat-type competition models with time delay and pulse in a polluted environment. *Journal of Mathematical Chemistry*, 47(1):123–144, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9536-2`.

Fujita:2010:CDS

[1585] Shinsaku Fujita. Correlation diagrams of stereoisograms for characterizing stereoisomers of cyclobutane derivatives. *Journal of Mathematical Chemistry*, 47(1):145–166, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9539-z`.

Karimi:2010:CGA

[1586] Sasan Karimi, Anthony Delgado, and Marty Lewinter. A combinatorial/geometric analysis of convex cyclofusene. *Journal of Mathematical Chemistry*, 47(1):167–173, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9538-0`.

Laszlo:2010:MCM

[1587] Tarko Laszlo. Monte Carlo method for identification of outlier molecules in QSAR studies. *Journal of Mathematical Chemistry*, 47(1):174–190, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9540-6`.

Puida:2010:MMA

[1588] Mantas Puida, Feliksas Ivanauskas, and Valdas Laurinavicius. Mathematical modeling of the action of biosensor possessing variable parame-

ters. *Journal of Mathematical Chemistry*, 47(1):191–200, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9541-5`.

Zhou:2010:RRW

[1589] Bo Zhou, Yong Yang, and Nenad Trinajstić. On reciprocal reverse Wiener index. *Journal of Mathematical Chemistry*, 47(1):201–209, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9543-3`.

Zhou:2010:GSC

[1590] Bo Zhou and Nenad Trinajstić. On general sum-connectivity index. *Journal of Mathematical Chemistry*, 47(1):210–218, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9542-4`.

Hudelson:2010:VTI

[1591] Matthew Hudelson. Vertex topological indices and tree expressions, generalizations of continued fractions. *Journal of Mathematical Chemistry*, 47(1):219–228, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9565-x`.

Milani:2010:OVE

[1592] G. Milani and F. Milani. Optimal vulcanization of 2D–3D EPM/EPDM thick elements through peroxidic mixtures. *Journal of Mathematical Chemistry*, 47(1):229–267, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9566-9`.

Zhou:2010:RDD

[1593] Bo Zhou and Nenad Trinajstić. On reverse degree distance. *Journal of Mathematical Chemistry*, 47(1):268–275, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9568-7`.

Teng:2010:GBM

[1594] Zhidong Teng, Rong Gao, Mehbuba Rehim, and Kai Wang. Global behaviors of Monod type chemostat model with nutrient recycling and impulsive input. *Journal of Mathematical Chemistry*, 47(1):276–294, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9567-8`.

Guseinov:2010:ACO

[1595] I. I. Guseinov, B. A. Mamedov, and Z. Andiç. Application of combined open shell Hartree–Fock–Roothaan theory to molecules using symmetrical one-range addition theorems of Slater type orbitals. *Journal of Mathematical Chemistry*, 47(1):295–304, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9569-6`.

Ilic:2010:EIC

[1596] Aleksandar Ilić and Dragan Stevanović. The Estrada index of chemical trees. *Journal of Mathematical Chemistry*, 47(1):305–314, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9570-0`.

Kosti:2010:OER

[1597] A. A. Kosti, Z. A. Anastassi, and T. E. Simos. An optimized explicit Runge–Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 47(1):315–330, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9571-z`.

Carbo-Dorca:2010:DNC

[1598] Ramon Carbó-Dorca. Definition of norm coherent generalized scalar products and quantum similarity. *Journal of Mathematical Chemistry*, 47 (1):331–344, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9572-y`.

Mamedov:2010:CTC

[1599] B. A. Mamedov and E. Çopuroğlu. Calculation of three-center nuclear attraction integral over Slater type orbitals in molecular coordinate system using Löwdin α-radial function and Guseinov's two-center charge density expansion formulae. *Journal of Mathematical Chemistry*, 47(1): 345–353, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9577-6`. See erratum [1600].

Mamedov:2010:ECT

[1600] B. A. Mamedov and E. Çopuroğlu. Erratum: Calculation of three-center nuclear attraction integral over Slater type orbitals in molecular coordinate system using Löwdin α-radial function and Guseinov's two-center

charge density expansion formulae. *Journal of Mathematical Chemistry*, 47(1):354, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9601-x; http://link.springer.com/content/pdf/10.1007/s10910-009-9601-x.pdf`. See [1599].

Toropov:2010:UIC

[1601] Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Danuta Leszczynska, and Jerzy Leszczynski. Use of the international chemical identifier for constructing QSPR-model of normal boiling points of acyclic carbonyl substances. *Journal of Mathematical Chemistry*, 47(1): 355–369, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9574-9`.

Dabulyte-Bagdonaviciene:2010:CTE

[1602] J. Dabulyte-Bagdonaviciene and F. Ivanauskas. The comparison of two electrochemical process models involving chemical steps. *Journal of Mathematical Chemistry*, 47(1):370–383, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9576-7`.

Guseinov:2010:EFTa

[1603] I. I. Guseinov. Expansion formulae for two-center charge densities of integer and noninteger n generalized exponential type orbitals applied to evaluation of multicenter multielectron integrals. *Journal of Mathematical Chemistry*, 47(1):384–390, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9578-5`.

Guseinov:2010:CTT

[1604] I. I. Guseinov. Combined theory of two- and four-component complete orthonormal sets of spinor wave functions and Slater type spinor orbitals in position, momentum and four-dimensional spaces. *Journal of Mathematical Chemistry*, 47(1):391–402, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9582-9`.

Helton:2010:SPC

[1605] J. William Helton, Vitaly Katsnelson, and Igor Klep. Sign patterns for chemical reaction networks. *Journal of Mathematical Chemistry*, 47 (1):403–429, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9579-4`.

Simelevicius:2010:CMA

[1606] Dainius Simelevicius and Romas Baronas. Computational modelling of amperometric biosensors in the case of substrate and product inhibition. *Journal of Mathematical Chemistry*, 47(1):430–445, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9581-x`.

Belov:2010:LPA

[1607] G. Belov. On linear programming approach for the calculation of chemical equilibrium in complex thermodynamic systems. *Journal of Mathematical Chemistry*, 47(1):446–456, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9580-y`.

Yang:2010:BL

[1608] Weiling Yang, Fuji Zhang, and Douglas J. Klein. Benzenoid links. *Journal of Mathematical Chemistry*, 47(1):457–476, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9583-8`.

Fath-Tabar:2010:NGA

[1609] Gholamhossein Fath-Tabar, Boris Furtula, and Ivan Gutman. A new geometric-arithmetic index. *Journal of Mathematical Chemistry*, 47(1):477–486, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9584-7`.

Tarko:2010:ECH

[1610] Laszlo Tarko and Mihai V. Putz. On electronegativity and chemical hardness relationships with aromaticity. *Journal of Mathematical Chemistry*, 47(1):487–495, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9585-6`.

Wei:2010:ECE

[1611] Shouliu Wei and Xiaoling Ke. Elementary components of essentially disconnected polyomino graphs. *Journal of Mathematical Chemistry*, 47(1):496–504, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9589-2`.

Niehaus:2010:CID

[1612] Thomas A. Niehaus, N. H. March, and S. Suhai. Correlated and idempotent Dirac first-order density matrices with identical diagonal Fermion density: a route to extract a one-body potential energy in TDDFT. *Journal of Mathematical Chemistry*, 47(1):505–519, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9592-7`.

March:2010:SMM

[1613] N. H. March and Z. D. Zhang. Statistical-mechanical models with separable many-body interactions: especially partition functions and thermodynamic consequences. *Journal of Mathematical Chemistry*, 47(1): 520–538, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9575-8`.

Yilmaz:2010:SSE

[1614] Hale Yilmaz, Dogan Demirhan, and Fevzi Büyükkiliç. Solution of the Schrödinger equation for two q-deformed potentials by the SWKB method. *Journal of Mathematical Chemistry*, 47(1):539–547, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9588-3`.

Carbo-Dorca:2010:MSP

[1615] Ramon Carbó-Dorca. A monodimensional scientific performance measure: the h index, can be substituted by simple multidimensional descriptors? *Journal of Mathematical Chemistry*, 47(1):548–550, January 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9573-x`.

Szederkenyi:2010:CSD

[1616] Gábor Szederkényi. Computing sparse and dense realizations of reaction kinetic systems. *Journal of Mathematical Chemistry*, 47(2):551–568, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9525-5`.

Lee:2010:SND

[1617] Richard K. F. Lee, Barry J. Cox, and James M. Hill. Silicon nanotubes with distinct bond lengths. *Journal of Mathematical Chemistry*, 47(2): 569–589, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9586-5.

Max:2010:ITE

[1618] Jean-Joseph Max and Camille Chapados. Infrared transmission equations in a five media system: gas and liquid. *Journal of Mathematical Chemistry*, 47(2):590–625, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9587-4.

Nicholson:2010:PFI

[1619] Victor A. Nicholson. Protein folding invariants. *Journal of Mathematical Chemistry*, 47(2):626–635, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9590-9.

deSousa:2010:ENC

[1620] A. G. de Sousa, A. B. F. da Silva, and V. S. Bagnato. The effect of the negative coupling parameter on the spectrum of a trapped Bose gas. *Journal of Mathematical Chemistry*, 47(2):636–646, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9591-8.

Toropov:2010:QAD

[1621] A. A. Toropov, A. P. Toropova, E. Benfenati, D. Leszczynska, and J. Leszczynski. QSAR analysis of 1,4-dihydro-4-oxo-1-(2-thiazolyl)-1,8-naphthyridines exhibiting anticancer activity by optimal SMILES-based descriptors. *Journal of Mathematical Chemistry*, 47(2):647–666, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9593-6.

Nalewajski:2010:UNA

[1622] Roman F. Nalewajski. Use of non-additive information measures in exploring molecular electronic structure: Stockholder bonded atoms and role of kinetic energy in the chemical bond. *Journal of Mathematical Chemistry*, 47(2):667–691, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9594-5.

Nalewajski:2010:MOP

[1623] Roman F. Nalewajski. Many-orbital probabilities and their entropy/information descriptors in orbital communication theory of the chemical bond. *Journal of Mathematical Chemistry*, 47(2):692–708, February

2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9595-4.

Nalewajski:2010:ANA

[1624] Roman F. Nalewajski. Additive and non-additive information channels in orbital communication theory of the chemical bond. *Journal of Mathematical Chemistry*, 47(2):709–738, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9596-3.

Wang:2010:HBM

[1625] Siyuan Wang, Xuncheng Huang, Lemin Zhu, and Minaya Villasana. Hopf bifurcation and multiple limit cycles in bio-chemical reaction of the morphogenesis process. *Journal of Mathematical Chemistry*, 47(2):739–749, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9597-2.

Lee:2010:RMM

[1626] Chang Hyeong Lee and Roger Lui. A reduction method for multiple time scale stochastic reaction networks with non-unique equilibrium probability. *Journal of Mathematical Chemistry*, 47(2):750–770, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9598-1.

Kardos:2010:CEC

[1627] Frantisek Kardos, Matjaz Krnc, Borut Luzar, and Riste Skrekovski. Cyclic 7-edge-cuts in fullerene graphs. *Journal of Mathematical Chemistry*, 47(2):771–789, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9599-0.

Ajadi:2010:ACC

[1628] S. O. Ajadi and O. Nave. Approximate critical conditions in thermal explosion theory for a two-step kinetic model. *Journal of Mathematical Chemistry*, 47(2):790–807, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9600-y.

Nalewajski:2010:EIC

[1629] Roman F. Nalewajski. Entropy/information coupling between orbital-communications in molecular subsystems. *Journal of Mathematical*

Chemistry, 47(2):808–832, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9602-9`.

Yuan:2010:GAI

[1630] Yan Yuan, Bo Zhou, and Nenad Trinajstić. On geometric-arithmetic index. *Journal of Mathematical Chemistry*, 47(2):833–841, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9603-8`.

Du:2010:MSC

[1631] Zhibin Du, Bo Zhou, and Nenad Trinajstić. Minimum sum-connectivity indices of trees and unicyclic graphs of a given matching number. *Journal of Mathematical Chemistry*, 47(2):842–855, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9604-7`.

Arimoto:2010:PFCa

[1632] Shigeru Arimoto. Proof of the Fukui conjecture via resolution of singularities and related methods: III. *Journal of Mathematical Chemistry*, 47 (2):856–870, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9605-6`.

Konguetsof:2010:NTS

[1633] A. Konguetsof. A new two-step hybrid method for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 47(2): 871–890, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9606-5`.

Meloun:2010:ODS

[1634] Milan Meloun, Sylva Bordovská, and Karel Kupka. Outliers detection in the statistical accuracy test of a pK_a prediction. *Journal of Mathematical Chemistry*, 47(2):891–909, February 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9609-2`.

Omiste:2010:ITP

[1635] J. J. Omiste, R. J. Yáñez, and J. S. Dehesa. Information-theoretic properties of the half-line Coulomb potential. *Journal of Mathematical Chemistry*, 47(3):911–928, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9611-8`.

Killingbeck:2010:NNI

[1636] J. P. Killingbeck and G. Jolicard. The Niblack–Nigam iterative method revisited. *Journal of Mathematical Chemistry*, 47(3):929–936, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9615-4`.

Wang:2010:OTM

[1637] Wen-Huan Wang and Li-Ying Kang. Ordering of the trees by minimal energies. *Journal of Mathematical Chemistry*, 47(3):937–958, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9616-3`.

Yukalov:2010:EIA

[1638] V. I. Yukalov, E. P. Yukalova, and S. Gluzman. Extrapolation and interpolation of asymptotic series by self-similar approximants. *Journal of Mathematical Chemistry*, 47(3):959–983, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9618-1`.

Lim:2010:MMP

[1639] Teik-Cheng Lim. Modification of Morse potential in conventional force fields for applying FPDP parameters. *Journal of Mathematical Chemistry*, 47(3):984–989, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9619-0`.

Berberan-Santos:2010:BFI

[1640] Mario N. Berberan-Santos, Evgeny N. Bodunov, and Lionello Pogliani. On the barometric formula inside the Earth. *Journal of Mathematical Chemistry*, 47(3):990–1004, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9620-7`.

Petrov:2010:ARR

[1641] Vesselin Petrov and Fernando Pina. Analytical resolution of the reaction rates of flavylium network by Laplace transform. *Journal of Mathematical Chemistry*, 47(3):1005–1026, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9621-6`.

Killingbeck:2010:GEM

[1642] John P. Killingbeck and Alain Grosjean. A Gauss elimination method for resonances. *Journal of Mathematical Chemistry*, 47(3):1027–1037, April

2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9622-5.

Urdiales:2010:FPE

[1643] E. Urdiales and Vladimir A. Volpert. Frontal polymerization with encapsulated monomer. *Journal of Mathematical Chemistry*, 47(3):1038–1053, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9623-4.

Yao:2010:NAN

[1644] Huanmin Yao. New algorithm for the numerical solution of the integro-differential equation with an integral boundary condition. *Journal of Mathematical Chemistry*, 47(3):1054–1067, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9628-z.

Nalewajski:2010:DEE

[1645] Roman F. Nalewajski. N-dependence of electronic energies in atoms and molecules: Mulliken and exponential interpolations. *Journal of Mathematical Chemistry*, 47(3):1068–1076, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9630-5.

Chuang:2010:CHD

[1646] Chern Chuang and Bih-Yaw Jin. Classification of hypothetical doubly and triply periodic porous graphitic structures by tilings of neck-like units. *Journal of Mathematical Chemistry*, 47(3):1077–1084, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9632-3.

Pongor:2010:DIS

[1647] Gábor Pongor, János Eőri, János Rohonczy, and Zsuzsanna Kolos. Direct inversion in the spectral subspace: A novel method for quantitative and qualitative analysis of chemical mixtures. *Journal of Mathematical Chemistry*, 47(3):1085–1105, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9633-2.

Lente:2010:CBS

[1648] Gábor Lente. The connection between the second law of thermodynamics and the principle of microscopic reversibility. *Journal of Mathematical*

Chemistry, 47(3):1106–1111, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9634-1`.

Zheng:2010:GCI

[1649] Jie Zheng. The general connectivity indices of catacondensed hexagonal systems. *Journal of Mathematical Chemistry*, 47(3):1112–1120, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9639-9`.

Sereni:2010:SPF

[1650] Jean-Sébastien Sereni and Matej Stehlík. On the sextet polynomial of fullerenes. *Journal of Mathematical Chemistry*, 47(3):1121–1128, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9640-3`.

Liu:2010:NMA

[1651] Yanqiu Liu and Yusen Zhang. A new method for analyzing H5N1 avian influenza virus. *Journal of Mathematical Chemistry*, 47(3):1129–1144, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9641-2`.

Vodopivec:2010:TDM

[1652] Andrej Vodopivec, Forrest H. Kaatz, and Bohan Mohar. Topographical distance matrices for porous arrays. *Journal of Mathematical Chemistry*, 47(3):1145–1153, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9651-0`. See erratum [1672].

Lu:2010:OIS

[1653] Lili Lu. Optimal inputs and sensitivities for parameter estimation in bioreactors. *Journal of Mathematical Chemistry*, 47(3):1154–1176, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9610-9`.

Balaban:2010:NPR

[1654] Alexandru T. Balaban. Nonconvex polyhedra by repeated truncation of semiregular polyhedra. *Journal of Mathematical Chemistry*, 47(3): 1177–1183, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9613-6.

Berberan-Santos:2010:MBI

[1655] Mário N. Berberan-Santos. Mathematical basis of the integral formalism of chemical kinetics. Compact representation of the general solution of the first-order linear differential equation. *Journal of Mathematical Chemistry*, 47(3):1184–1188, April 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9631-4.

Zhao:2010:DAL

[1656] Zhong Zhao and Lansun Chen. Dynamic analysis of lactic acid fermentation with impulsive input. *Journal of Mathematical Chemistry*, 47(4):1189–1208, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-008-9494-0.

Klein:2010:CMG

[1657] D. J. Klein. Centrality measure in graphs. *Journal of Mathematical Chemistry*, 47(4):1209–1223, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9635-0.

Zhao:2010:ISF

[1658] Zhong Zhao, Li Yang, and Lansun Chen. Impulsive state feedback control of the microorganism culture in a turbidostat. *Journal of Mathematical Chemistry*, 47(4):1224–1239, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9644-z.

Guseinov:2010:EII

[1659] I. I. Guseinov. Evaluation of intermolecular interaction energy using one-range addition theorems for ψ^{α}-ETO and Coulomb–Yukawa like correlated interaction potentials with integer and noninteger indices. *Journal of Mathematical Chemistry*, 47(4):1240–1247, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9645-y; http://link.springer.com/content/pdf/10.1007/s10910-009-9645-y.pdf.

Hasanov:2010:ANI

[1660] Alemdar Hasanov, Burhan Pektas, and Umit Kadiroglu. An analysis of nonlinear ion transport problem including arbitrary valences of oxi-

dized and reduced species. *Journal of Mathematical Chemistry*, 47(4): 1248–1262, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9649-7`.

Ahmad:2010:MCI

[1661] Tahir Ahmad, Sabariah Baharun, and Khairil Anuar Arshad. Modeling a clinical incineration process using fuzzy autocatalytic set. *Journal of Mathematical Chemistry*, 47(4):1263–1273, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9650-1`.

Tuvi-Arad:2010:DSC

[1662] Inbal Tuvi-Arad and David Avnir. Determining symmetry changes during a chemical reaction: the case of diazene isomerization. *Journal of Mathematical Chemistry*, 47(4):1274–1286, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9653-y`.

Sellers:2010:TBR

[1663] Peter H. Sellers. Torsion in biochemical reaction networks. *Journal of Mathematical Chemistry*, 47(4):1287–1302, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9654-x`.

Gutman:2010:TPE

[1664] Ivan Gutman. Theory of the PCP effect and related phenomena. *Journal of Mathematical Chemistry*, 47(4):1303–1312, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9655-9`.

Glasser:2010:EET

[1665] M. L. Glasser, N. H. March, and L. M. Nieto. Exchange energy for two closed shells generated by a bare Coulomb potential energy $-Ze^2/r$ in the limit of large Z, in two dimensions. *Journal of Mathematical Chemistry*, 47(4):1313–1322, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9656-8`.

Altay:2010:NSO

[1666] Nejla Altay and Metin Demiralp. Numerical solution of ordinary differential equations by fluctuationlessness theorem. *Journal of Mathematical*

Chemistry, 47(4):1323–1343, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9657-7`.

Miranda-Quintana:2010:FTC

[1667] Ramón-Alain Miranda-Quintana, Roberto Cruz-Rodes, Edelsys Codorniu-Hernandez, and Alfo José Batista-Leyva. Formal theory of the comparative relations: its application to the study of quantum similarity and dissimilarity measures and indices. *Journal of Mathematical Chemistry*, 47(4):1344–1365, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9658-6`.

Belkic:2010:RTI

[1668] Dzevad Belkić. Review of theories on ionization in fast ion–atom collisions with prospects for applications to hadron therapy. *Journal of Mathematical Chemistry*, 47(4):1366–1419, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9662-x`.

Belkic:2010:RTD

[1669] Dzevad Belkić. Review of theories on double electron capture in fast ion–atom collisions. *Journal of Mathematical Chemistry*, 47(4):1420–1467, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9663-9`.

Strekalov:2010:TTW

[1670] M. L. Strekalov. A treatment of the torsional wave equation with an internal rotation constant depending on a torsional angle via point canonical transformation. *Journal of Mathematical Chemistry*, 47(4):1468–1475, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9617-2`.

Gligor:2010:NMS

[1671] Delia Maria Gligor and Mihaela Ligia Unguresan. Numerical modelling and simulation of Laviron treatment for poly-phenothiazine derivative-modified glassy carbon electrodes. *Journal of Mathematical Chemistry*, 47(4):1476–1482, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9629-y`.

Vodopivec:2010:ETD

[1672] Andrej Vodopivec, Forrest H. Kaatz, and Bojan Mohar. Erratum to: Topographical distance matrices for porous arrays. *Journal of Mathematical Chemistry*, 47(4):1483, May 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9672-8; http://link.springer.com/content/pdf/10.1007/s10910-010-9672-8.pdf`. See [1652].

Vigo-Aguiar:2010:MCT

[1673] J. Vigo-Aguiar and E. J. Brändas. Mathematical and computational tools in theoretical chemistry. *Journal of Mathematical Chemistry*, 48(1):1–2, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9612-7; http://link.springer.com/content/pdf/10.1007/s10910-009-9612-7.pdf`.

Alonso:2010:NEE

[1674] P. Alonso, J. Delgado, R. Gallego, and J. M. Peña. Neville elimination: an efficient algorithm with application to chemistry. *Journal of Mathematical Chemistry*, 48(1):3–20, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9648-8`.

Perez-Garcia:2010:SAC

[1675] M. Ángeles Pérez-García. Shape analysis of clusterized neutron rich matter. *Journal of Mathematical Chemistry*, 48(1):21–27, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9608-3`.

Bayon:2010:IGS

[1676] L. Bayón, J. M. Grau, M. M. Ruiz, and P. M. Suárez. Initial guess of the solution of dynamic optimization of chemical processes. *Journal of Mathematical Chemistry*, 48(1):28–37, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9614-5`.

Ramos:2010:NSNa

[1677] Higinio Ramos, J. Vigo-Aguiar, S. Natesan, R. García-Rubio, and M. A. Queiruga. Numerical solution of nonlinear singularly perturbed problems on nonuniform meshes by using a non-standard algorithm. *Journal of Mathematical Chemistry*, 48(1):38–54, July 2010. CODEN JM-

CHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9625-2`.

Rizea:2010:EFM

[1678] M. Rizea. Exponential fitting method for the time-dependent Schrödinger equation. *Journal of Mathematical Chemistry*, 48(1):55–65, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9626-1`.

Guirao:2010:PEC

[1679] Juan Luis García Guirao and Marek Lampart. Positive entropy of a coupled lattice system related with Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 48(1):66–71, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9624-3`.

Ala:2010:MAE

[1680] G. Ala, E. Francomano, A. Spagnuolo, and A. Tortorici. A meshless approach for electromagnetic simulation of metallic carbon nanotubes. *Journal of Mathematical Chemistry*, 48(1):72–77, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9627-0`.

Ghiringhelli:2010:ITA

[1681] Luca M. Ghiringhelli, Luigi Delle Site, Ricardo A. Mosna, and I. P. Hamilton. Information-theoretic approach to kinetic-energy functionals: the nearly uniform electron gas. *Journal of Mathematical Chemistry*, 48(1):78–82, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9690-6`.

denHollander:2010:MMC

[1682] F. den Hollander and N. Pétrélis. A mathematical model for a copolymer in an emulsion. *Journal of Mathematical Chemistry*, 48(1):83–94, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9564-y; http://link.springer.com/content/pdf/10.1007/s10910-009-9564-y.pdf`.

Alonso:2010:MCM

[1683] Pedro Alonso, Ian P. Hamilton, and J. Vigo-Aguiar. Mathematical and computational methods with applications in chemistry and physics. *Journal of Mathematical Chemistry*, 48(1):95–97, July

2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9661-y; http://link.springer.com/content/pdf/10.1007/s10910-010-9661-y.pdf.

Ramos:2010:NSNb

[1684] Higinio Ramos and R. García-Rubio. Numerical solution of nonlinear singularly perturbed problems by using a non-standard algorithm on variable stepsize implementation (CMMSE-2009). *Journal of Mathematical Chemistry*, 48(1):98–108, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9636-z.

Laurrabaquio:2010:TFA

[1685] Guadalupe López Laurrabaquio, M. Begoña Torres, Eva. M. Fernández, and L. Carlos Balbás. Trends in the formation of aggregates and crystals from M@Si_{16} clusters: a study from first principle calculations. *Journal of Mathematical Chemistry*, 48(1):109–117, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9637-y.

Escobedo:2010:OCC

[1686] Ramón Escobedo and Luis A. Fernández. Optimal control of chemical birth and growth processes in a deterministic model. *Journal of Mathematical Chemistry*, 48(1):118–127, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9638-x.

DiBlasi:2010:ENB

[1687] G. Di Blasi, E. Francomano, A. Tortorici, and E. Toscano. Exploiting numerical behaviors in SPH. *Journal of Mathematical Chemistry*, 48 (1):128–136, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9642-1.

Yeguas:2010:CSS

[1688] Violeta Yeguas, Gloria Inés Cárdenas-Jirón, María Isabel Menéndez, and Ramón López. A computational study on the stability-aromaticity correlation of triply N-confused porphyrins: CMMSE-09. *Journal of Mathematical Chemistry*, 48(1):137–144, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-009-9643-0.

Lima:2010:NMO

[1689] Pedro M. Lima and Luisa Morgado. Numerical modeling of oxygen diffusion in cells with Michaelis–Menten uptake kinetics. *Journal of Mathematical Chemistry*, 48(1):145–158, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9646-x`.

Guirao:2010:CCL

[1690] Juan Luis García Guirao and Marek Lampart. Chaos of a coupled lattice system related with the Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 48(1):159–164, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9647-9`.

Rey-Ronco:2010:MSI

[1691] M. A. Rey-Ronco, T. Alonso-Sánchez, and M. P. Castro-García. Mathematical study to improve the sensitivity in the neutron activation analysis of fluorspar. *Journal of Mathematical Chemistry*, 48(1):165–174, July 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9652-z`.

Berberan-Santos:2010:GFM

[1692] Mário N. Berberan-Santos. Green's function method and the first-order linear differential equation. *Journal of Mathematical Chemistry*, 48(2):175–178, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9678-2`.

Meena:2010:MME

[1693] A. Meena, A. Eswari, and L. Rajendran. Mathematical modelling of enzyme kinetics reaction mechanisms and analytical solutions of non-linear reaction equations. *Journal of Mathematical Chemistry*, 48(2):179–186, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-009-9659-5`.

Zhao:2010:ASC

[1694] Xuezhuang Zhao, Zhenfeng Shang, Zucheng Li, Xiufang Xu, Guichang Wang, Ruifang Li, and Yun Li. Approximate symmetry characteristics using fuzzy-subset theory study for chiral transitions of allene-1,3,-dihalides. *Journal of Mathematical Chemistry*, 48(2):187–223, August

2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9660-z.

Konguetsof:2010:TSH

[1695] A. Konguetsof. Two-step high order hybrid explicit method for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 48(2):224–252, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9664-8.

Altinbasak:2010:SLMa

[1696] Sevda Üsküplü Altinbasak and Metin Demiralp. Solutions to linear matrix ordinary differential equations via minimal, regular, and excessive space extension based universalization. *Journal of Mathematical Chemistry*, 48(2):253–265, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9665-7.

Altinbasak:2010:SLMb

[1697] Sevda Üsküplü Altinbasak and Metin Demiralp. Solutions to linear matrix ordinary differential equations via minimal, regular, and excessive space extension based universalization. *Journal of Mathematical Chemistry*, 48(2):266–286, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9667-5.

Kristensen:2010:TTQ

[1698] Thomas G. Kristensen. Transforming Tanimoto queries on real valued vectors to range queries in Euclidian space. *Journal of Mathematical Chemistry*, 48(2):287–289, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9668-4.

Kazantzis:2010:ADB

[1699] Nikolaos Kazantzis, Vasiliki Kazantzi, and Emmanuel G. Christodoulou. On aspects of the dynamic behavior of persistent chemicals in a multimedia environment related to exposure-based hazard assessment. *Journal of Mathematical Chemistry*, 48(2):290–304, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9669-3.

Haus:2010:DRN

[1700] Utz-Uwe Haus and Raymond Hemmecke. Decomposition of reaction networks: the initial phase of the permanganate/oxalic acid reaction. *Journal of Mathematical Chemistry*, 48(2):305–312, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9670-x`.

Dias:2010:SFI

[1701] Jerry Ray Dias. Structure/formula informatics of isomeric sets of fluoranthenoid/fluorenoid and indacenoid hydrocarbons. *Journal of Mathematical Chemistry*, 48(2):313–329, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9671-9`.

Li:2010:GLZ

[1702] Chun Li, Zhengxing Li, Xiaoqi Zheng, Hong Ma, and Xiaoqing Yu. A generalization of Lempel–Ziv complexity and its application to the comparison of protein sequences. *Journal of Mathematical Chemistry*, 48 (2):330–338, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9673-7`.

dOnofrio:2010:UGA

[1703] Alberto d'Onofrio. Uniqueness and global attractivity of glycolytic oscillations suggested by Selkov's model. *Journal of Mathematical Chemistry*, 48(2):339–346, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9674-6`.

Munoz-Munoz:2010:NFS

[1704] Jose Luis Muñoz-Muñoz, Francisco Garcia-Molina, Ramón Varon, Jose Tudela, Francisco Garcia-Cánovas, and Jose N. Rodríguez-López. New features of the steady-state rate related with the initial concentration of substrate in the diphenolase and monophenolase activities of tyrosinase. *Journal of Mathematical Chemistry*, 48(2):347–362, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9675-5`.

Lim:2010:AKP

[1705] Teik-Cheng Lim. Application of Kihara parameters in conventional molecular force fields. *Journal of Mathematical Chemistry*, 48(2): 363–369, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9676-4.

Furtula:2010:AZI

[1706] Boris Furtula, Ante Graovac, and Damir Vukicević. Augmented Zagreb index. *Journal of Mathematical Chemistry*, 48(2):370–380, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9677-3.

Gibson:2010:FAS

[1707] David R. Gibson and Hari Pulapaka. A fast algorithm and software for analysis of FT–ICR data. *Journal of Mathematical Chemistry*, 48 (2):381–394, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9679-1.

Vukicevic:2010:OTD

[1708] Damir Vukicević, Marin Bralo, Ana Klarić, Antonija Markovina, Dina Spahija, Ana Tadić, and Ana Zilić. One-two descriptor. *Journal of Mathematical Chemistry*, 48(2):395–400, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9681-7.

Hu:2010:CPA

[1709] Guang Hu, Wen-Yuan Qiu, Xiao-Sheng Cheng, and Shu-Ya Liu. The complexity of platonic and Archimedean polyhedral links. *Journal of Mathematical Chemistry*, 48(2):401–412, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9682-6. See erratum [1755].

Hasanov:2010:IUDa

[1710] Alemdar Hasanov. Identification of unknown diffusion and convection coefficients in ion transport problems from flux data: an analytical approach. *Journal of Mathematical Chemistry*, 48(2):413–423, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9683-5.

Zhang:2010:UEG

[1711] Dongfang Zhang. On the unimolecular elimination of gas-phase iodine monobromide following excitation in the visible wavelength region. *Journal of Mathematical Chemistry*, 48(2):424–438, August 2010. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9684-4.

Liu:2010:APL

[1712] Shu-Ya Liu, Xiao-Sheng Cheng, Heping Zhang, and Wen-Yuan Qiu. The architecture of polyhedral links and their HOMFLY polynomials. *Journal of Mathematical Chemistry*, 48(2):439–456, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9685-3.

Barabas:2010:SAA

[1713] B. Barabás, J. Tóth, and G. Pályi. Stochastic aspects of asymmetric autocatalysis and absolute asymmetric synthesis. *Journal of Mathematical Chemistry*, 48(2):457–489, August 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9680-8.

Hasanov:2010:IUDb

[1714] Alemdar Hasanov. Identification of unknown diffusion coefficient in pure diffusive linear model of chronoamperometry. I. The theory. *Journal of Mathematical Chemistry*, 48(3):491–507, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9686-2.

Hasanov:2010:IUDc

[1715] Alemdar Hasanov and Burhan Pektas. Identification of unknown diffusion coefficient in pure diffusive linear model of chronoamperometry. II. Numerical implementation. *Journal of Mathematical Chemistry*, 48(3):508–520, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9687-1.

Natarajan:2010:NCD

[1716] R. Natarajan, R. Jayalakshmi, and M. Vivekanandan. Numerical characterization of DNA sequences: connectivity type indices derived from DNA line graphs. *Journal of Mathematical Chemistry*, 48(3):521–529, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9688-0.

Milani:2010:NSN

[1717] G. Milani and F. Milani. A new simple numerical model based on experimental scorch curve data fitting for the interpretation of sulphur

vulcanization. *Journal of Mathematical Chemistry*, 48(3):530–557, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9689-z`.

Mansour:2010:TWP

[1718] M. B. A. Mansour. Traveling wave patterns in nonlinear reaction-diffusion equations. *Journal of Mathematical Chemistry*, 48(3):558–565, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9691-5`.

Stadler:2010:MGC

[1719] Adrian-Mihail Stadler. Molecular geometry and conformation: mathematical relations between intra-molecular distances and conformation in Fréchet-type dendrimers and dendrons. *Journal of Mathematical Chemistry*, 48(3):566–582, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9692-4`.

Xing:2010:SCI

[1720] Rundan Xing, Bo Zhou, and Nenad Trinajstić. Sum-connectivity index of molecular trees. *Journal of Mathematical Chemistry*, 48(3):583–591, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9693-3`.

Quina:2010:CDS

[1721] P. L. Dammig Quiña, V. E. Pastor, I. M. Irurzun, and E. E. Mola. Configurational degeneracy of a set of dipoles in a quasi-two-dimensional system. *Journal of Mathematical Chemistry*, 48(3):592–600, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9694-2`.

Safouhi:2010:IPC

[1722] Hassan Safouhi. Integrals of the paramagnetic contribution in the relativistic calculation of the shielding tensor. *Journal of Mathematical Chemistry*, 48(3):601–616, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9695-1`.

Masia-Perez:2010:GMNa

[1723] J. Masiá-Pérez, J. Escribano, E. Valero, E. Arribas, M. García-Moreno, J. L. Muñoz-Muñoz, R. Gómez-Ladrón de Guevara, and R. Varón. A

general model for non-autocatalytic zymogen activation in the presence of two different and mutually exclusive inhibitors. I. Kinetic analysis. *Journal of Mathematical Chemistry*, 48(3):617–634, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9696-0`.

Masia-Perez:2010:GMNb

[1724] J. Masiá-Pérez, J. Escribano, E. Valero, E. Arribas, M. García-Moreno, J. L. Muñoz-Muñoz, R. Gómez-Ladrón de Guevara, and R. Varón. A general model for non-autocatalytic zymogen activation in the presence of two different and mutually exclusive inhibitors. II. Relative weight of activation and inhibition processes. *Journal of Mathematical Chemistry*, 48 (3):635–652, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9697-z`.

Qin:2010:ABD

[1725] Wenjie Qin and Zhijun Liu. Asymptotic behaviors of a delay difference system of plankton allelopathy. *Journal of Mathematical Chemistry*, 48 (3):653–675, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9698-y`.

Shiu:2010:MRC

[1726] Wai Chee Shiu, Heping Zhang, and Saihua Liu. Maximal resonance of cubic bipartite polyhedral graphs. *Journal of Mathematical Chemistry*, 48 (3):676–686, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9700-8`.

deSousa:2010:ODT

[1727] A. G. de Sousa, A. B. F. da Silva, and V. S. Bagnato. One-dimensional trapped atoms: critical coupling parameter and critical number of particles. *Journal of Mathematical Chemistry*, 48(3):687–696, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9701-7`.

Du:2010:MGS

[1728] Zhibin Du, Bo Zhou, and Nenad Trinajstić. Minimum general sum-connectivity index of unicyclic graphs. *Journal of Mathematical Chemistry*, 48(3):697–703, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9702-6`.

Cheng:2010:DAE

[1729] Yi Cheng, Yanchun Li, Shi Yan, and Chuan Huang. Deviation of activation energy caused by neglecting a temperature term in Ozawa equation. *Journal of Mathematical Chemistry*, 48(3):704–713, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9703-5`.

Zhou:2010:SPR

[1730] Bo Zhou and Nenad Trinajstić. Some properties of the reformulated Zagreb indices. *Journal of Mathematical Chemistry*, 48(3):714–719, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9704-4`.

Zhang:2010:MSA

[1731] Haitao Zhang, Zaihang Zheng, Xuejun Cui, Hongyan Wang, and Mei Han. Multi-scales association modeling of membrane water resistance indexes. *Journal of Mathematical Chemistry*, 48(3):720–732, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9705-3`.

Zhang:2010:CCN

[1732] Heping Zhang, Dong Ye, and Yunrui Liu. A combination of Clar number and Kekulé count as an indicator of relative stability of fullerene isomers of C_{60}. *Journal of Mathematical Chemistry*, 48(3):733–740, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9706-2`.

Tikhonov:2010:OCD

[1733] Nikolai A. Tikhonov. Oscillations of the concentration during sorption of amino acids on ion exchanger grains. *Journal of Mathematical Chemistry*, 48(3):741–751, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9707-1`.

Nalewajski:2010:EGC

[1734] R. F. Nalewajski. Electronic-geometric coupling in model reactive system. *Journal of Mathematical Chemistry*, 48(3):752–775, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9708-0`.

Arimoto:2010:PFCb

[1735] Shigeru Arimoto, Mark Spivakovsky, Keith F. Taylor, and Paul G. Mezey. Proof of the Fukui conjecture via resolution of singularities and related methods. IV. *Journal of Mathematical Chemistry*, 48(3):776–790, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9709-z`.

Chen:2010:VJD

[1736] Goong Chen, Zhonghai Ding, Chang-Shou Lin, Dudley Herschbach, and Marlan O. Scully. Variational justification of the dimensional-scaling method in chemical physics: the h-atom. *Journal of Mathematical Chemistry*, 48(3):791–811, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9710-6`.

Guseinov:2010:EFTb

[1737] I. I. Guseinov. Expansion formulae for two-center charge densities of integer and noninteger n generalized exponential type orbitals with hyperbolic cosine and their use in evaluation of multicenter multielectron integrals. *Journal of Mathematical Chemistry*, 48(3):812–815, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9711-5`.

Bucknum:2010:T

[1738] Michael J. Bucknum, Bin Wen, and Eduardo A. Castro. Trigohexagonite. *Journal of Mathematical Chemistry*, 48(3):816–826, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9713-3`.

Tunga:2010:ISF

[1739] Burcu Tunga and Metin Demiralp. The influence of the support functions on the quality of enhanced multivariance product representation. *Journal of Mathematical Chemistry*, 48(3):827–840, October 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9714-2`.

Dutt:2010:TPA

[1740] A. K. Dutt. Turing pattern amplitude equation for a model glycolytic reaction-diffusion system. *Journal of Mathematical Chemistry*, 48(4): 841–855, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9699-x; http://www.springerlink.com/content/e04jmlj1q418p52k/.

Huber:2010:NTD

[1741] Alfred Huber. A new time dependent approach for solving electrochemical interfaces. Part I: theoretical considerations using Lie group analysis. *Journal of Mathematical Chemistry*, 48(4):856–875, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9712-4.

Zhang:2010:ESN

[1742] Min-Cang Zhang, Bo An, and Huang-Fu Guo-Qing. Exact solutions of a new Coulomb ring-shaped potential. *Journal of Mathematical Chemistry*, 48(4):876–882, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9715-1.

Gluzman:2010:SSE

[1743] S. Gluzman and V. I. Yukalov. Self-similar extrapolation from weak to strong coupling. *Journal of Mathematical Chemistry*, 48(4):883–913, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9716-0.

Carbo-Dorca:2010:GHT

[1744] Ramon Carbó-Dorca and Emili Besalú. A Gaussian holographic theorem and the projection of electronic density functions into the surface of a sphere. *Journal of Mathematical Chemistry*, 48(4):914–924, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9717-z.

Alolyan:2010:HAO

[1745] Ibraheem Alolyan and T. E. Simos. High algebraic order methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 48(4):925–958, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9718-y.

Toropova:2010:QMM

[1746] Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati, Danuta Leszczynska, and Jerzy Leszczynski. QSAR modeling of measured bind-

ing affinity for fullerene-based HIV-1 PR inhibitors by CORAL. *Journal of Mathematical Chemistry*, 48(4):959–987, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9719-x`.

Koga:2010:EPR

[1747] Toshikatsu Koga and Masahiro Sekiya. Electron-pair radial density functions. *Journal of Mathematical Chemistry*, 48(4):988–1000, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9720-4`.

Delgado:2010:SEN

[1748] Víctor Delgado. The Sherman equations as a nonlinear Perron eigenvalue problem. *Journal of Mathematical Chemistry*, 48(4):1001–1009, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9721-3`.

Li:2010:DMR

[1749] Genyuan Li and Herschel Rabitz. D-MORPH regression: application to modeling with unknown parameters more than observation data. *Journal of Mathematical Chemistry*, 48(4):1010–1035, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9722-2`.

Killingbeck:2010:PAF

[1750] J. P. Killingbeck and A. Lakhlifi. A perturbation approach to finite difference methods. *Journal of Mathematical Chemistry*, 48(4):1036–1043, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9723-1`.

Hariharan:2010:HWM

[1751] G. Hariharan and K. Kannan. Haar wavelet method for solving some nonlinear parabolic equations. *Journal of Mathematical Chemistry*, 48(4):1044–1061, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9724-0`.

Mateljevic:2010:EPC

[1752] Miodrag Mateljević, Vladimir Bozin, and Ivan Gutman. Energy of a polynomial and the Coulson integral formula. *Journal of Mathematical*

Chemistry, 48(4):1062–1068, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9725-z`.

Ghosh:2010:CPA

[1753] Piyali Ghosh and Bholanath Mandal. Characteristic polynomials of alternant edge weighted linear chains with subsequent application to some linear poly (p-phenylene) graphs. *Journal of Mathematical Chemistry*, 48(4):1069–1091, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9726-y`.

Alolyan:2010:MMV

[1754] Ibraheem Alolyan and T. E. Simos. Mulitstep methods with vanished phase-lag and its first and second derivatives for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 48(4):1092–1143, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9728-9`.

Hu:2010:ECP

[1755] Guang Hu, Wen-Yuan Qiu, Xiao-Sheng Cheng, and Shu-Ya Liu. Erratum to: The complexity of Platonic and Archimedean polyhedral links. *Journal of Mathematical Chemistry*, 48(4):1144, November 2010. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9727-x; http://link.springer.com/content/pdf/10.1007/s10910-010-9727-x.pdf`. See [1709].

Varga:2011:RDF

[1756] Stefan Varga. On robust density fitting in molecules and extended systems. *Journal of Mathematical Chemistry*, 49(1):1–5, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9736-9`.

Ayers:2011:RBE

[1757] Paul W. Ayers and Ramon Carbó-Dorca. The relationship between the eigenvalues and eigenvectors of a similarity matrix and its associated Carbó index matrix. *Journal of Mathematical Chemistry*, 49(1):6–11, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9737-8`.

Lee:2011:MUW

[1758] Young Lee, Donald J. Kouri, and David K. Hoffman. Minimum uncertainty wavelets in non-relativistic super-symmetric quantum mechanics. *Journal of Mathematical Chemistry*, 49(1):12–34, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9729-8`.

Zivkovic:2011:ETG

[1759] Tomislav P. Zivković. Exact treatment of generalized modifications of finite-dimensional systems by the LRM approach. *Journal of Mathematical Chemistry*, 49(1):35–78, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9730-2`.

Jablan:2011:TJP

[1760] S. Jablan, Lj. Radović, and R. Sazdanović. Tutte and Jones polynomials of links, polyominoes and graphical recombination patterns. *Journal of Mathematical Chemistry*, 49(1):79–94, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9731-1`.

Fujita:2011:TOS

[1761] Shinsaku Fujita. Theory of organic stereoisomerism in harmony with molecular symmetry. *Journal of Mathematical Chemistry*, 49(1):95–162, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9732-0`.

Canedo:2011:KAM

[1762] M. M. Canedo and J. L. González-Hernández. KINMODEL (AGDC): a multipurpose computational method for kinetic treatment. *Journal of Mathematical Chemistry*, 49(1):163–184, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9733-z`.

Basak:2011:QSA

[1763] Subhash C. Basak and D. Mills. Quantitative structure-activity relationship studies of boron-containing dipeptide proteasome inhibitors using calculated mathematical descriptors. *Journal of Mathematical Chemistry*, 49(1):185–200, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9734-y`.

Mamedov:2011:UBC

[1764] B. A. Mamedov and E. Çopuroğlu. Use of binomial coefficients in fast and accurate calculation of Löwdin-alpha radial functions. *Journal of Mathematical Chemistry*, 49(1):201–207, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9735-x`.

Jeanniton:2011:QTS

[1765] Juan R. Jeanniton. Quantum transition state theory: featuring ensemble pre-equilibrium approximation. *Journal of Mathematical Chemistry*, 49 (1):208–240, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9742-y`.

Strekalov:2011:BTP

[1766] M. L. Strekalov. Building transition probabilities per collision from transition rates per unit time for finding the mean observable quantities in the gas phase. *Journal of Mathematical Chemistry*, 49(1):241–250, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9743-x`.

Velkovsky:2011:MMC

[1767] Momchil Velkovsky, Rachel Snider, David E. Cliffel, and John P. Wikswo. Modeling the measurements of cellular fluxes in microbioreactor devices using thin enzyme electrodes. *Journal of Mathematical Chemistry*, 49 (1):251–275, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9744-9`.

Mozrzymas:2011:PCM

[1768] Anna Mozrzymas and Bozenna Rózycka-Roszak. Prediction of critical micelle concentration of cationic surfactants using connectivity indices. *Journal of Mathematical Chemistry*, 49(1):276–289, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9738-7; http://link.springer.com/content/pdf/10.1007/s10910-010-9738-7.pdf`.

Guseinov:2011:EPE

[1769] I. I. Guseinov. Evaluation of potential of electric field produced by molecule using symmetrical one-range addition theorems for Coulomb–

Yukawa like correlated interaction potentials of integer and noninteger indices. *Journal of Mathematical Chemistry*, 49(1):290–295, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9739-6`.

Champagnat:2011:RAM

[1770] Nicolas Champagnat, Chris Chipot, and Erwan Faou. Reconciling alternate methods for the determination of charge distributions: a probabilistic approach to high-dimensional least-squares approximations. *Journal of Mathematical Chemistry*, 49(1):296–324, January 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9740-0`.

Zhang:2011:ZOG

[1771] Minjie Zhang and Shuchao Li. On the zeroth-order general Randić index. *Journal of Mathematical Chemistry*, 49(2):325–327, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9759-2`.

Williams:2011:AST

[1772] Brian Wesley Williams. Alternate solutions for two particular third order kinetic rate laws. *Journal of Mathematical Chemistry*, 49(2):328–334, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9765-4`.

March:2011:EED

[1773] N. H. March, A. Krishtal, C. Van Alsenoy, and J. D. Talman. Exchange energy density definitions from the optimized exchange-force, exemplified for non-relativistic Ne- and Ar-like atomic ions in the limit of large nuclear charge. *Journal of Mathematical Chemistry*, 49(2):335–341, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9741-z`.

Shanmugasundaram:2011:ASL

[1774] Veerabahu Shanmugasundaram and Gerald M. Maggiora. Application of Shannon-like diversity measures to cell-based chemistry spaces. *Journal of Mathematical Chemistry*, 49(2):342–355, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9745-8`.

Lepore:2011:CMC

[1775] Dante M. Lepore, Carl Barratt, and Pauline M. Schwartz. Computational models of chemical systems inspired by Braess' paradox. *Journal of Mathematical Chemistry*, 49(2):356–370, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9746-7`.

Nalewajski:2011:TST

[1776] Roman F. Nalewajski. Through-space and through-bridge components of chemical bonds. *Journal of Mathematical Chemistry*, 49(2):371–392, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9747-6; http://link.springer.com/content/pdf/10.1007/s10910-010-9747-6.pdf`.

Baykara:2011:FAN

[1777] N. A. Baykara, Ercan Gürvit, and Metin Demiralp. The fluctuationlessness approach to the numerical integration of functions with a single variable by integrating Taylor expansion with explicit remainder term. *Journal of Mathematical Chemistry*, 49(2):393–406, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9748-5`.

Kursunlu:2011:FRBa

[1778] Aysegül Kursunlu and Metin Demiralp. A fluctuation removal based univariate integration over prescribed nodes: certain important aspects of one node fluctuation free integration. *Journal of Mathematical Chemistry*, 49(2):407–427, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9749-4`.

Kursunlu:2011:FRBb

[1779] Aysegül Kursunlu and Metin Demiralp. A fluctuation removal based univariate integration over prescribed nodes. *Journal of Mathematical Chemistry*, 49(2):428–443, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9750-y`.

Gao:2011:MRT

[1780] Hui Gao and Yan Fu. Mean residence time of Markov processes for particle transport in fluidized bed reactors. *Journal of Mathematical Chemistry*, 49(2):444–456, February 2011. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9751-x.

Rahamathunissa:2011:MNB

[1781] G. Rahamathunissa, P. Manisankar, L. Rajendran, and K. Venugopal. Modeling of nonlinear boundary value problems in enzyme-catalyzed reaction diffusion processes. *Journal of Mathematical Chemistry*, 49(2): 457–474, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9752-9.

Baowan:2011:MJN

[1782] Duangkamon Baowan, Barry J. Cox, and James M. Hill. Modelling the joining of nanocones and nanotubes. *Journal of Mathematical Chemistry*, 49(2):475–488, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9753-8.

Zhifang:2011:SCE

[1783] Liu Zhifang and C. Rongsi. The structure character of essentially disconnected polyomino graphs. *Journal of Mathematical Chemistry*, 49(2): 489–506, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9754-7.

Wang:2011:QST

[1784] Yaoxiong Wang, Rebing Wu, Xin Chen, Yunjian Ge, Junhui Shi, Herschel Rabitz, and Feng Shuang. Quantum state transformation by optimal projective measurements. *Journal of Mathematical Chemistry*, 49(2): 507–519, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9755-6.

Ozalp:2011:UCC

[1785] Nuri Ozalp and Elgiz Bairamov. Uniform convergence and computation of the generalized exponential integrals. *Journal of Mathematical Chemistry*, 49(2):520–530, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9756-5.

dOnofrio:2011:GAO

[1786] Alberto d'Onofrio. Globally attractive oscillations in open monosubstrate allosteric enzyme reactions. *Journal of Mathematical Chemistry*, 49(2):

531–545, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9757-4.

Nalewajski:2011:CBT

[1787] Roman F. Nalewajski. Chemical bonds from through-bridge orbital communications in prototype molecular systems. *Journal of Mathematical Chemistry*, 49(2):546–561, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9761-8; http://link.springer.com/content/pdf/10.1007/s10910-010-9761-8.pdf.

Szczepanik:2011:EBD

[1788] Dariusz Szczepanik and Janusz Mrozek. Entropic bond descriptors from separated output-reduced communication channels in atomic orbital resolution. *Journal of Mathematical Chemistry*, 49(2):562–575, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9763-6; http://link.springer.com/content/pdf/10.1007/s10910-010-9763-6.pdf.

Yildirim:2011:RAB

[1789] Necmettin Yildirim and Jonathan K. Statz. Response analysis in biochemical chain reactions with negative feedforward and feedbackward loops. *Journal of Mathematical Chemistry*, 49(2):576–591, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9764-5.

Nalewajski:2011:UBP

[1790] Roman F. Nalewajski. Use of the bond-projected superposition principle in determining the conditional probabilities of orbital events in molecular fragments. *Journal of Mathematical Chemistry*, 49(2):592–608, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9766-3; http://link.springer.com/content/pdf/10.1007/s10910-010-9766-3.pdf.

Ergun:2011:ENH

[1791] Ebru Ergun and Elgiz Bairamov. On the eigenvalues of a 3 by 3 non-Hermitian Hamiltonian. *Journal of Mathematical Chemistry*, 49(2):609–617, February 2011. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9767-2.

Carbo-Dorca:2011:LKD

[1792] Ramon Carbó-Dorca. Logical Kronecker delta deconstruction of the absolute value function and the treatment of absolute deviations. *Journal of Mathematical Chemistry*, 49(3):619–624, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9781-4.

Cohen:2011:GEG

[1793] Leon Cohen. On the generalization of the Edgeworth/Gram–Charlier series. *Journal of Mathematical Chemistry*, 49(3):625–628, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9787-y.

Tikhonov:2011:MML

[1794] N. A. Tikhonov and M. G. Tokmachev. Mathematical modelling of low-frequency oscillations in solute transport by diffusion through a membrane. *Journal of Mathematical Chemistry*, 49(3):629–642, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9758-3.

Banerji:2011:MCO

[1795] Anirban Banerji and Indira Ghosh. Mathematical criteria to observe mesoscopic emergence of protein biochemical properties. *Journal of Mathematical Chemistry*, 49(3):643–665, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9760-9.

Chaves:2011:IPT

[1796] J. Chaves, J. M. Barroso, and E. Besalú. An iterative perturbation theory with a Hamiltonian modifier. *Journal of Mathematical Chemistry*, 49 (3):666–686, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9762-7.

Altay:2011:HDM

[1797] Nejla Altay and Metin Demiralp. A high dimensional model representation based numerical method for solving ordinary differential equations. *Journal of Mathematical Chemistry*, 49(3):687–710, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9768-1.

Alolyan:2011:FES

[1798] Ibraheem Alolyan and T. E. Simos. A family of eight-step methods with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 49 (3):711–764, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9773-4`.

Qian:2011:OEB

[1799] Ailin Qian and Yan Li. Optimal error bound and generalized Tikhonov regularization for identifying an unknown source in the heat equation. *Journal of Mathematical Chemistry*, 49(3):765–775, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9774-3`.

Bersani:2011:MAD

[1800] A. M. Bersani, E. Bersani, and L. Mastroeni. Modeling the action of drugs on cellular enzymes by means of optimal control techniques. *Journal of Mathematical Chemistry*, 49(3):776–795, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9775-2`.

Luo:2011:QSC

[1801] Hua-Jun Luo, Jun-Zhi Wang, and Kun Zou. QSAR study on cytotoxic activity (against KB cells) of some hederagenin diglycosides using support vector regression. *Journal of Mathematical Chemistry*, 49 (3):796–805, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9776-1`.

Nalewajski:2011:IOC

[1802] Roman F. Nalewajski. On interference of orbital communications in molecular systems. *Journal of Mathematical Chemistry*, 49(3): 806–815, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9777-0; http://link.springer.com/content/pdf/10.1007/s10910-010-9777-0.pdf`.

Zhang:2011:CEA

[1803] Z. D. Zhang and N. H. March. Are the critical exponents for Anderson localization due to disorder well understood? *Journal of Mathematical*

Chemistry, 49(3):816–820, March 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9778-z`.

Cassam-Chenai:2011:RSP

[1804] P. Cassam-Chenaï. Rayleigh–Schrödinger perturbation theory generalized to eigen-operators in non-commutative rings. *Journal of Mathematical Chemistry*, 49(4):821–835, April 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9779-y`.

Carbo-Dorca:2011:MAL

[1805] R. Carbó-Dorca and E. Besalú. Mathematical aspects of the LCAO MO first order density function (4): a discussion on the connection of Taylor series expansion of electronic density (TSED) function with the holographic electron density theorem (HEDT) and the Hohenberg–Kohn theorem (HKT). *Journal of Mathematical Chemistry*, 49(4):836–842, April 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9780-5`.

Sikiric:2011:CPR

[1806] Mathieu Dutour Sikirić and Patrick W. Fowler. Cubic polyhedral Ramanujan graphs with face size no larger than six. *Journal of Mathematical Chemistry*, 49(4):843–858, April 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9782-3`.

Benson:2011:SAS

[1807] James D. Benson. Stability analysis of several non-dilute multiple solute transport equations. *Journal of Mathematical Chemistry*, 49(4):859–869, April 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9783-2`.

Calogero:2011:NRE

[1808] F. Calogero, F. Leyvraz, and M. Sommacal. Novel rate equations describing isochronous chemical reactions. *Journal of Mathematical Chemistry*, 49(4):870–879, April 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9784-1`.

Arimoto:2011:FNS

[1809] Shigeru Arimoto. Fundamental notions for the second generation Fukui project and a prototypal problem of the normed repeat space and its super spaces. *Journal of Mathematical Chemistry*, 49(4):880–893, April 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9785-0`.

Tunga:2011:FFM

[1810] Burcu Tunga and Metin Demiralp. Fluctuation free multivariate integration based logarithmic HDMR in multivariate function representation. *Journal of Mathematical Chemistry*, 49(4):894–909, April 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9786-z`.

Imada:2011:EES

[1811] Tomoki Imada, Shunsuke Ota, Hiroshi Nagamochi, and Tatsuya Akutsu. Efficient enumeration of stereoisomers of tree structured molecules using dynamic programming. *Journal of Mathematical Chemistry*, 49(4): 910–970, April 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9789-9`.

Lopez-Rosa:2011:PMI

[1812] S. López-Rosa, J. Montero, P. Sánchez-Moreno, J. Venegas, and J. S. Dehesa. Position and momentum information-theoretic measures of a D-dimensional particle-in-a-box. *Journal of Mathematical Chemistry*, 49(5):971–994, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9790-3`.

Baronas:2011:MCN

[1813] Romas Baronas, Juozas Kulys, Karolis Petrauskas, and Julija Razumiene. Modelling carbon nanotube based biosensor. *Journal of Mathematical Chemistry*, 49(5):995–1010, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9791-2`.

Guseinov:2011:UTC

[1814] I. I. Guseinov. Unified treatment of complex and real rotation-angular functions for two-center overlap integrals over arbitrary atomic orbitals.

Journal of Mathematical Chemistry, 49(5):1011–1013, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9792-1`.

Aygar:2011:PTD

[1815] Yelda Aygar and Elgiz Bairamov. Properties of the two-dimensional exponential integral functions. *Journal of Mathematical Chemistry*, 49 (5):1014–1025, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9793-0`.

Zheng:2011:SDM

[1816] Hao Zheng and Weimin Han. On some discretization methods for solving a linear matrix ordinary differential equation. *Journal of Mathematical Chemistry*, 49(5):1026–1041, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9794-z`.

Baowan:2011:MME

[1817] Duangkamon Baowan, Kittisak Chayantrakom, Pairote Satiracoo, and Barry J. Cox. Mathematical modelling for equilibrium configurations of concentric gold nanoparticles. *Journal of Mathematical Chemistry*, 49 (5):1042–1053, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9796-x`.

Gubernov:2011:PIZ

[1818] V. V. Gubernov, A. V. Kolobov, A. A. Polezhaev, and H. S. Sidhu. Pulsating instabilities in the Zeldovich–Liñán model. *Journal of Mathematical Chemistry*, 49(5):1054–1070, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9797-9`.

Szalkai:2011:CMR

[1819] Balázs Szalkai and István Szalkai. Counting minimal reactions with specific conditions in $\mathbf{r}^4$. *Journal of Mathematical Chemistry*, 49(5): 1071–1085, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9798-8`.

Lim:2011:AER

[1820] Teik-Cheng Lim. Application of extended-Rydberg parameters in general Morse potential functions. *Journal of Mathematical Chemistry*, 49(5):

1086–1091, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-010-9799-7.

Tunga:2011:MBI

[1821] M. Alper Tunga. A matrix based indexing HDMR method for multivariate data modelling. *Journal of Mathematical Chemistry*, 49(5): 1092–1114, May 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9800-0.

Tran-Duc:2011:OBM

[1822] Thien Tran-Duc, Ngamta Thamwattana, and James M. Hill. Orientation of a benzene molecule inside a carbon nanotube. *Journal of Mathematical Chemistry*, 49(6):1115–1127, June 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9809-4.

Tian:2011:TPC

[1823] Canrong Tian. Turing patterns created by cross-diffusion for a Holling II and Leslie–Gower type three species food chain model. *Journal of Mathematical Chemistry*, 49(6):1128–1150, June 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9801-z; http://www.springerlink.com/content/e34638060128n170/.

Puida:2011:MEC

[1824] Mantas Puida, Albertas Malinauskas, and Feliksas Ivanauskas. Modeling of electrocatalysis at conducting polymer modified electrodes: nonlinear current-concentration profiles. *Journal of Mathematical Chemistry*, 49 (6):1151–1162, June 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9802-y.

Szederkenyi:2011:FCB

[1825] Gábor Szederkényi and Katalin M. Hangos. Finding complex balanced and detailed balanced realizations of chemical reaction networks. *Journal of Mathematical Chemistry*, 49(6):1163–1179, June 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9804-9.

Lim:2011:SSP

[1826] Teik-Cheng Lim. Split series potential energy function. *Journal of Mathematical Chemistry*, 49(6):1180–1191, June 2011. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9806-7.

Baker:2011:CIE

[1827] A. David Baker, Mark D. Baker, and Christopher R. H. Hanusa. Corner ion, edge-center ion, and face-center ion Madelung expressions for sodium chloride. *Journal of Mathematical Chemistry*, 49(6):1192–1198, June 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9807-6.

Li:2011:FST

[1828] Yun Li, Shengkai Xing, Xuezhuang Zhao, Zhenfeng Shang, Zunsheng Cai, Xiufang Xu, Guichang Wang, and Ruifang Li. Fuzzy symmetries of two classes of linear polyacene molecules. *Journal of Mathematical Chemistry*, 49(6):1199–1216, June 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9808-5.

Zoboki:2011:SPA

[1829] Tamás Zoboki and Péter R. Surján. A stationary property of the APSG wave function. *Journal of Mathematical Chemistry*, 49(7):1217–1225, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9833-4.

Nalewajski:2011:IBD

[1830] Roman F. Nalewajski and Piotr Gurdek. On the implicit bond-dependency origins of bridge interactions. *Journal of Mathematical Chemistry*, 49(7):1226–1237, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9815-6; http://link.springer.com/content/pdf/10.1007/s10910-011-9815-6.pdf.

Klein:2011:PGG

[1831] Douglas J. Klein and Vladimir R. Rosenfeld. Phased graphs and graph energies. *Journal of Mathematical Chemistry*, 49(7):1238–1244, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9814-7.

Klein:2011:PC

[1832] Douglas J. Klein and Vladimir R. Rosenfeld. Phased cycles. *Journal of Mathematical Chemistry*, 49(7):1245–1255, August 2011. CODEN JM-

CHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9813-8.

Klein:2011:DG

[1833] Douglas J. Klein and Vladimir R. Rosenfeld. Dinormal graphs. *Journal of Mathematical Chemistry*, 49(7):1256–1262, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9812-9.

Johnston:2011:LCC

[1834] Matthew D. Johnston and David Siegel. Linear conjugacy of chemical reaction networks. *Journal of Mathematical Chemistry*, 49(7):1263–1282, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9817-4.

Zhang:2011:TTD

[1835] Z. D. Zhang and N. H. March. Temperature-time duality exemplified by Ising magnets and quantum-chemical many electron theory. *Journal of Mathematical Chemistry*, 49(7):1283–1290, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9820-9.

Liu:2011:FME

[1836] Yuli Liu and Paul W. Ayers. Finding minimum energy reaction paths on ab initio potential energy surfaces using the fast marching method. *Journal of Mathematical Chemistry*, 49(7):1291–1301, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9818-3.

Schulze-Halberg:2011:TDD

[1837] Axel Schulze-Halberg. Two-dimensional Darboux transformations for non-separable angular equations and solvable non-central potentials. *Journal of Mathematical Chemistry*, 49(7):1302–1310, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9829-0.

Restrepo:2011:PDN

[1838] Guillermo Restrepo and Douglas J. Klein. Predicting densities of nitrocubanes using partial orders. *Journal of Mathematical Chemistry*, 49(7):1311–1321, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9834-3.

Tasi:2011:ANC

[1839] Gyula Tasi and Dóra Barna. Analytical and numerical computation of error propagation of model parameters. *Journal of Mathematical Chemistry*, 49(7):1322–1329, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9830-7`.

Konguetsof:2011:HMP

[1840] A. Konguetsof. A hybrid method with phase-lag and derivatives equal to zero for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 49(7):1330–1356, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9824-5`.

Milani:2011:EAS

[1841] G. Milani and F. Milani. EPDM accelerated sulfur vulcanization: a kinetic model based on a genetic algorithm. *Journal of Mathematical Chemistry*, 49(7):1357–1383, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9832-5`.

Jesudason:2011:NNA

[1842] Christopher G. Jesudason. I. Numerical nonlinear analysis: differential methods and optimization applied to chemical reaction rate determination. *Journal of Mathematical Chemistry*, 49(7):1384–1415, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9831-6`.

Sharifi:2011:RGI

[1843] Hesam Sharifi. Rational groups and integer-valued characters of Thompson group Th. *Journal of Mathematical Chemistry*, 49(7):1416–1423, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9837-0`.

Senent:2011:ISS

[1844] M. L. Senent. Ab initio spectroscopic studies of non-rigid molecules: an application to acetic acid. *Journal of Mathematical Chemistry*, 49(7):1424–1435, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9836-1`.

Szmytkowski:2011:DAL

[1845] Radosław Szmytkowski. On the derivative of the associated Legendre function of the first kind of integer order with respect to its degree (with applications to the construction of the associated Legendre function of the second kind of integer degree and order). *Journal of Mathematical Chemistry*, 49(7):1436–1477, August 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9826-3; http://link.springer.com/content/pdf/10.1007/s10910-011-9826-3.pdf`.

Huang:2011:PAD

[1846] Yujuan Huang and Tianming Wang. Phylogenetic analysis of DNA sequences with a novel characteristic vector. *Journal of Mathematical Chemistry*, 49(8):1479–1492, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9811-x`.

Rogerson:2011:MSS

[1847] Parker Rogerson and Gustavo A. Arteca. Molecular size scaling in families of protein native folds. *Journal of Mathematical Chemistry*, 49(8):1493–1506, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9825-4`.

Santosa:2011:IPR

[1848] Fadil Santosa and Benjamin Weitz. An inverse problem in reaction kinetics. *Journal of Mathematical Chemistry*, 49(8):1507–1520, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9835-2`.

Baronas:2011:MCS

[1849] Darius Baronas, Feliksas Ivanauskas, and Romas Baronas. Mechanisms controlling the sensitivity of amperometric biosensors in flow injection analysis systems. *Journal of Mathematical Chemistry*, 49(8):1521–1534, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9838-z`.

Marmorino:2011:ELB

[1850] M. G. Marmorino. Eigenvalue lower bounds with Bazley's special choice of an infinite-dimensional subspace. *Journal of Mathematical Chem-*

istry, 49(8):1535–1543, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9839-y`.

Monaco:2011:NDC

[1851] Guglielmo Monaco. A novel derivation of collision theory rate constants for a bimolecular reaction. *Journal of Mathematical Chemistry*, 49(8):1544–1557, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9840-5`.

Mercado:2011:QSD

[1852] Luz Dary Mercado and Ramon Carbó-Dorca. Quantum similarity and discrete representation of molecular sets. *Journal of Mathematical Chemistry*, 49(8):1558–1572, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9841-4`.

Gaidamauskaite:2011:MSA

[1853] Evelina Gaidamauskaite, Romas Baronas, and Juozas Kulys. Modelling synergistic action of laccase-based biosensor utilizing simultaneous substrates conversion. *Journal of Mathematical Chemistry*, 49(8):1573–1586, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9844-1`.

Yang:2011:NNG

[1854] Yujun Yang, Heping Zhang, and Douglas J. Klein. New Nordhaus–Gaddum-type results for the Kirchhoff index. *Journal of Mathematical Chemistry*, 49(8):1587–1598, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9845-0`.

Panin:2011:PAE

[1855] A. I. Panin. Polynomial approximations of electronic wave functions. *Journal of Mathematical Chemistry*, 49(8):1599–1623, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9846-z`.

Fernandez:2011:NAS

[1856] J. R. Fernández and M. C. Muñiz. Numerical analysis of surfactant dynamics at air-water interface using the Henry isotherm. *Journal of Mathematical Chemistry*, 49(8):1624–1645, September 2011. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9847-y.

Yuan:2011:DIO

[1857] Sanling Yuan, Pan Li, and Yongli Song. Delay induced oscillations in a turbidostat with feedback control. *Journal of Mathematical Chemistry*, 49(8):1646–1666, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9848-x.

Arribas:2011:CUE

[1858] E. Arribas, J. M. Villalba, M. Garcia-Moreno, M. L. Amo, F. Garcia-Sevilla, F. Garcia-Molina, J. L. Muñoz-Muñoz, and R. Varon. Characterization of unstable enzyme systems which evolve according to a three-exponential equation. *Journal of Mathematical Chemistry*, 49(8): 1667–1686, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9850-3.

Roy:2011:DFC

[1859] Amlan K. Roy. Density functional calculation of many-electron systems in Cartesian coordinate grid. *Journal of Mathematical Chemistry*, 49(8): 1687–1699, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9851-2.

Arimoto:2011:PFC

[1860] Shigeru Arimoto, Mark Spivakovsky, Eiji Yoshida, Keith F. Taylor, and Paul G. Mezey. Proof of the Fukui conjecture via resolution of singularities and related methods. V. *Journal of Mathematical Chemistry*, 49(8): 1700–1712, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9852-1.

Maheswari:2011:ASN

[1861] M. Uma Maheswari and L. Rajendran. Analytical solution of non-linear enzyme reaction equations arising in mathematical chemistry. *Journal of Mathematical Chemistry*, 49(8):1713–1726, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9853-0.

Thiagarajan:2011:AES

[1862] S. Thiagarajan, A. Meena, S. Anitha, and L. Rajendran. Analytical expression of the steady-state catalytic current of mediated bioelectrocatal-

ysis and the application of He's homotopy perturbation method. *Journal of Mathematical Chemistry*, 49(8):1727–1740, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9854-z`.

Sanchez:2011:NAA

[1863] S. Sánchez, F. Casas, and A. Fernández. New analytic approximations based on the Magnus expansion. *Journal of Mathematical Chemistry*, 49(8):1741–1758, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9855-y`.

Randic:2011:NCP

[1864] Milan Randić and Rok Orel. On numerical characterization of proteomics maps based on partitioning of 2-D maps into Voronoi regions. *Journal of Mathematical Chemistry*, 49(8):1759–1768, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9856-x`.

Besalu:2011:GGP

[1865] Emili Besalú and Ramon Carbó-Dorca. The general Gaussian product theorem. *Journal of Mathematical Chemistry*, 49(8):1769–1784, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9857-9`.

Zheng:2011:SSH

[1866] Hao Zheng and Weimin Han. On simplified spherical harmonics equations for the radiative transfer equation. *Journal of Mathematical Chemistry*, 49(8):1785–1797, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9858-8`.

Varga:2011:NIU

[1867] László Varga, Botond Szabó, István Gy. Zsély, András Zempléni, and Tamás Turányi. Numerical investigation of the uncertainty of Arrhenius parameters. *Journal of Mathematical Chemistry*, 49(8):1798–1809, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9859-7`.

Chakraborty:2011:FWK

[1868] Debajit Chakraborty and Paul W. Ayers. Failure of the Weizsäcker kinetic energy functional for one-, two-, and three-electron distribution

functions. *Journal of Mathematical Chemistry*, 49(8):1810–1821, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9860-1`.

Chakraborty:2011:AMS

[1869] Debajit Chakraborty and Paul W. Ayers. Assessment of the March–Santamaria kinetic energy pair-density functional. *Journal of Mathematical Chemistry*, 49(8):1822–1830, September 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9861-0`.

Aktas:2011:NBS

[1870] Metin Aktas. Novel bound states treatment of the two dimensional Schrödinger equation with pseudocentral potentials plus multiparameter noncentral potential. *Journal of Mathematical Chemistry*, 49(9): 1831–1842, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9873-9`.

Alolyan:2011:FTS

[1871] Ibraheem Alolyan and T. E. Simos. A family of ten-step methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 49(9): 1843–1888, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9862-z`.

Rohwedder:2011:ADA

[1872] Thorsten Rohwedder and Reinhold Schneider. An analysis for the DIIS acceleration method used in quantum chemistry calculations. *Journal of Mathematical Chemistry*, 49(9):1889–1914, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9863-y`.

Liu:2011:NTF

[1873] Yuli Liu, Steven K. Burger, and Paul W. Ayers. Newton trajectories for finding stationary points on molecular potential energy surfaces. *Journal of Mathematical Chemistry*, 49(9):1915–1927, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9864-x`.

Harbrecht:2011:ADG

[1874] Helmut Harbrecht. On analytical derivatives for geometry optimization in the polarizable continuum model. *Journal of Mathematical Chemistry*, 49(9):1928–1936, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9865-9`.

Das:2011:CSQ

[1875] Chandrachur Das and Kamal Bhattacharyya. Construction of stationary quantum states with targeted energies. *Journal of Mathematical Chemistry*, 49(9):1937–1948, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9866-8`.

Baleizao:2011:EKT

[1876] Carlos Baleizão and Mário N. Berberan-Santos. Enzyme kinetics with a twist. *Journal of Mathematical Chemistry*, 49(9):1949–1960, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9868-6`.

Barbosu:2011:TBP

[1877] Mihail Barbosu, Vasile Mioc, Daniel Pasca, and Ferenc Szenkovits. The two-body problem with generalized Lennard-Jones potential. *Journal of Mathematical Chemistry*, 49(9):1961–1975, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9867-7`.

ConceicaoBispo:2011:EKS

[1878] Jose Ailton Conceicao Bispo, Carlos Francisco Sampaio Bonafe, Volnei Brito de Souza, João Batista de Almeida e Silva, and Giovani Brandao Mafra de Carvalho. Extending the kinetic solution of the classic Michaelis–Menten model of enzyme action. *Journal of Mathematical Chemistry*, 49(9):1976–1995, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9869-5`.

Tunga:2011:CMB

[1879] Burcu Tunga and Metin Demiralp. Constancy maximization based weight optimization in high dimensional model representation for multivariate functions. *Journal of Mathematical Chemistry*, 49(9):1996–2012, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9870-z.

Bayanov:2011:NSV

[1880] I. M. Bayanov and R. Vanhaelst. The numerical simulation of vanadium RedOx flow batteries. *Journal of Mathematical Chemistry*, 49(9): 2013–2031, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9872-x.

Dey:2011:ONL

[1881] Bijoy K. Dey. Optimal non-linear dimension reduction scheme for classical molecular dynamics. *Journal of Mathematical Chemistry*, 49(9): 2032–2052, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9874-8.

Gu:2011:ESM

[1882] Xiao-Yan Gu and Shi-Hai Dong. Energy spectrum of the Manning–Rosen potential including centrifugal term solved by exact and proper quantization rules. *Journal of Mathematical Chemistry*, 49(9):2053–2062, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9877-5.

Jin:2011:AJP

[1883] Xian'an Jin and Fuji Zhang. The architecture and the Jones polynomial of polyhedral links. *Journal of Mathematical Chemistry*, 49(9): 2063–2088, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9876-6.

Liu:2011:CBT

[1884] Ying Liu, Bihui Liu, Yue Liu, and Michael G. B. Drew. Correlations between two sets of angular relation equations. *Journal of Mathematical Chemistry*, 49(9):2089–2108, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9875-7.

Carbo-Dorca:2011:QSV

[1885] Ramon Carbó-Dorca. Quantum similarity, volume functions and generalized Carbó indices. *Journal of Mathematical Chemistry*, 49(9):2109–2115, October 2011. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9878-4.

Gnacadja:2011:RPCa

[1886] Gilles Gnacadja. Reachability, persistence, and constructive chemical reaction networks (part i): reachability approach to the persistence of chemical reaction networks. *Journal of Mathematical Chemistry*, 49(10): 2117–2136, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9894-4.

Gnacadja:2011:RPCb

[1887] Gilles Gnacadja. Reachability, persistence, and constructive chemical reaction networks (part II): a formalism for species composition in chemical reaction network theory and application to persistence. *Journal of Mathematical Chemistry*, 49(10):2137–2157, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9896-2.

Gnacadja:2011:RPCc

[1888] Gilles Gnacadja. Reachability, persistence, and constructive chemical reaction networks (part III): a mathematical formalism for binary enzymatic networks and application to persistence. *Journal of Mathematical Chemistry*, 49(10):2158–2176, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9895-3.

Hogreve:2011:REB

[1889] H. Hogreve. Rigorous energy bounds for two-electron systems. *Journal of Mathematical Chemistry*, 49(10):2177–2189, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9879-3.

Chan:2011:DBM

[1890] Yue Chan and James M. Hill. Dynamics of benzene molecules situated in metal-organic frameworks. *Journal of Mathematical Chemistry*, 49(10): 2190–2209, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9880-x.

Falati:2011:ICS

[1891] M. Falati and G. Hojjati. Integration of chemical stiff ODEs using exponential propagation method. *Journal of Mathematical Chemistry*, 49(10):

2210–2230, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9881-9`.

Besalu:2011:DES

[1892] E. Besalú and R. Carbó-Dorca. n-Dimensional Euclidean space Gaussian enfoldment. *Journal of Mathematical Chemistry*, 49(10):2231–2243, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9882-8`.

Carbo-Dorca:2011:GDE

[1893] Ramon Carbó-Dorca and Emili Besalú. Geometry of n-dimensional Euclidean space Gaussian enfoldments. *Journal of Mathematical Chemistry*, 49(10):2244–2249, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9883-7`.

Jablan:2011:NGD

[1894] Slavik Jablan, Ljiljana Radović, and Radmila Sazdanović. Nonplanar graphs derived from Gauss codes of virtual knots and links. *Journal of Mathematical Chemistry*, 49(10):2250–2267, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9884-6`.

March:2011:SSC

[1895] N. H. March and Á. Nagy. Scaling of some chemical properties of tetrahedral and octahedral molecules plus almost spherical C and B cages. *Journal of Mathematical Chemistry*, 49(10):2268–2274, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9885-5`.

Anderson:2011:BTW

[1896] David F. Anderson. Boundedness of trajectories for weakly reversible, single linkage class reaction systems. *Journal of Mathematical Chemistry*, 49(10):2275–2290, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9886-4`.

Baowan:2011:MAW

[1897] D. Baowan and N. Thamwattana. Modelling adsorption of a water molecule into various pore structures of silica gel. *Journal of Mathematical Chemistry*, 49(10):2291–2307, November 2011. CODEN JM-

CHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9887-3.

Nalewajski:2011:EID

[1898] Roman F. Nalewajski. Entropy/information descriptors of the chemical bond revisited. *Journal of Mathematical Chemistry*, 49(10):2308–2329, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9888-2; http://link.springer.com/content/pdf/10.1007/s10910-011-9888-2.pdf.

Tarko:2011:NMU

[1899] Laszlo Tarko. A new manner to use application of Shannon entropy in similarity computation. *Journal of Mathematical Chemistry*, 49(10):2330–2344, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9889-1.

Bielinska-Waz:2011:GNR

[1900] Dorota Bielińska-Waz. Graphical and numerical representations of DNA sequences: statistical aspects of similarity. *Journal of Mathematical Chemistry*, 49(10):2345–2407, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9890-8; http://link.springer.com/content/pdf/10.1007/s10910-011-9890-8.pdf.

Belkic:2011:PPI

[1901] Dzevad Belkić and Karen Belkić. The potential for practical improvements in cancer diagnostics by mathematically-optimized magnetic resonance spectroscopy. *Journal of Mathematical Chemistry*, 49(10):2408–2440, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9891-7.

Haus:2011:RBC

[1902] Utz-Uwe Haus, Raymond Hemmecke, and Sebastian Pokutta. Reconstructing biochemical cluster networks. *Journal of Mathematical Chemistry*, 49(10):2441–2456, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9892-6.

Ruiz:2011:EHC

[1903] María Belén Ruiz. Evaluation of Hylleraas–CI atomic integrals. III. Two-electron kinetic energy integrals. *Journal of Mathematical Chemistry*, 49(10):2457–2485, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9893-5`.

Simos:2011:TSM

[1904] T. E. Simos. A two-step method with vanished phase-lag and its first two derivatives for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 49(10):2486–2518, November 2011. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9897-1`.

Csercsik:2012:PUD

[1905] Dávid Csercsik, Gábor Szederkényi, and Katalin M. Hangos. Parametric uniqueness of deficiency zero reaction networks. *Journal of Mathematical Chemistry*, 50(1):1–8, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9902-8`.

Dhatt:2012:ISW

[1906] Sharmistha Dhatt and Kamal Bhattacharyya. Infinite square well with a sinusoidal bottom: a candidate for the Klauder phenomenon? *Journal of Mathematical Chemistry*, 50(1):9–16, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9913-5`.

Weniger:2012:MNG

[1907] Ernst Joachim Weniger. On the mathematical nature of Guseinov's rearranged one-range addition theorems for Slater-type functions. *Journal of Mathematical Chemistry*, 50(1):17–81, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9914-4`.

Ajadi:2012:TEC

[1908] Suraju Olusegun Ajadi. Thermal explosion characteristics in a reduced kinetics model. *Journal of Mathematical Chemistry*, 50(1):82–98, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9871-y`.

Li:2012:GFH

[1909] Genyuan Li and Herschel Rabitz. General formulation of HDMR component functions with independent and correlated variables. *Journal of Mathematical Chemistry*, 50(1):99–130, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9898-0`.

Ke:2012:LBN

[1910] Xiaoling Ke. A lower bound on the number of elementary components of essentially disconnected generalized polyomino graphs. *Journal of Mathematical Chemistry*, 50(1):131–140, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9900-x`.

Skakauskas:2012:NSK

[1911] V. Skakauskas and P. Katauskis. Numerical study of the kinetics of unimolecular heterogeneous reactions onto planar surfaces. *Journal of Mathematical Chemistry*, 50(1):141–154, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9901-9`.

DAmbrosio:2012:PEE

[1912] Raffaele D'Ambrosio, Elena Esposito, and Beatrice Paternoster. Parameter estimation in exponentially fitted hybrid methods for second order differential problems. *Journal of Mathematical Chemistry*, 50(1): 155–168, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9903-7`.

Rogerson:2012:SSB

[1913] Parker Rogerson and Gustavo A. Arteca. Size scaling behaviour in protein domains belonging to the all-α, all-β, α/β, and $\alpha+\beta$ folding classes. *Journal of Mathematical Chemistry*, 50(1):169–186, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9904-6`.

Kessler:2012:EPC

[1914] Mathieu Kessler and José Pérez. Equivalence properties of the Cremer & Pople puckering coordinates for N-membered rings. *Journal of Mathematical Chemistry*, 50(1):187–209, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9905-5`.

Carbo-Dorca:2012:SPC

[1915] Ramon Carbó-Dorca and Emili Besalú. Shells, point cloud huts, generalized scalar products, cosines and similarity tensor representations in vector semispaces. *Journal of Mathematical Chemistry*, 50(1):210–219, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9906-4`.

Baas:2012:CSN

[1916] Nils A. Baas and Nadrian C. Seeman. On the chemical synthesis of new topological structures. *Journal of Mathematical Chemistry*, 50(1): 220–232, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9907-3`.

Corzo:2012:LDP

[1917] H. H. Corzo, H. G. Laguna, and R. P. Sagar. Localization-delocalization phenomena in a cyclic box. *Journal of Mathematical Chemistry*, 50(1): 233–248, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9908-2`. See comment [2785].

Miyazawa:2012:SSA

[1918] Tomotaka Miyazawa, Munehiro Aratake, and Susumu Onaka. Superspherical-shape approximation to describe the morphology of small crystalline particles having near-polyhedral shapes with round edges. *Journal of Mathematical Chemistry*, 50(1):249–260, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9909-1`.

Yang:2012:HRF

[1919] Rui Yang and Heping Zhang. Hexagonal resonance of (3,6)-fullerenes. *Journal of Mathematical Chemistry*, 50(1):261–273, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9910-8`.

Johnston:2012:LPA

[1920] Matthew D. Johnston, David Siegel, and Gábor Szederkényi. A linear programming approach to weak reversibility and linear conjugacy of chemical reaction networks. *Journal of Mathematical Chemistry*, 50 (1):274–288, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9911-7`.

Kanal:2012:TAI

[1921] M. E. Kanal, N. A. Baykara, and M. Demiralp. Theory and algorithm of the inversion method for pentadiagonal matrices. *Journal of Mathematical Chemistry*, 50(1):289–299, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9915-3`.

Baowan:2012:MCD

[1922] Duangkamon Baowan. Modelling of carbon dioxide: methane separation using titanium dioxide nanotubes. *Journal of Mathematical Chemistry*, 50(1):300–309, January 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9917-1`.

Vigo-Aguiar:2012:ACM

[1923] Jesús Vigo-Aguiar and Juan L. G. Guirao. Advances in computational and mathematical chemistry. *Journal of Mathematical Chemistry*, 50(2):311–312, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9805-8; http://link.springer.com/content/pdf/10.1007/s10910-011-9805-8.pdf`.

Escobedo:2012:OCS

[1924] Ramón Escobedo and Luis A. Fernández. Optimal cooling strategies in polymer crystallization. *Journal of Mathematical Chemistry*, 50(2):313–324, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9803-x`.

Rey-Ronco:2012:MNA

[1925] M. A. Rey-Ronco, T. Alonso-Sánchez, and M. P. Castro-García. Modeling of neutron activation process with americium beryllium source. Application to the activation of fluorspar samples. *Journal of Mathematical Chemistry*, 50(2):325–334, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9771-6`.

Bersani:2012:TAL

[1926] Alberto Maria Bersani and Guido Dell'Acqua. Is there anything left to say on enzyme kinetic constants and quasi-steady state approximation? *Journal of Mathematical Chemistry*, 50(2):335–344, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9770-7`.

Alonso:2012:ESB

[1927] P. Alonso, R. Cortina, J. Ranilla, and A. M. Vidal. An efficient and scalable block parallel algorithm of Neville elimination as a tool for the CMB maps problem. *Journal of Mathematical Chemistry*, 50(2): 345–358, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9769-0`.

Cumeras:2012:MPF

[1928] Raquel Cumeras, Isabel Gràcia, Eduard Figueras, Luis Fonseca, Joaquin Santander, Marc Salleras, Carlos Calaza, Neus Sabaté, and Carles Cané. Modelling a P-FAIMS with multiphysics FEM. *Journal of Mathematical Chemistry*, 50(2):359–373, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9772-5`.

Guirao:2012:DPR

[1929] Juan Luis García Guirao and María T. de Bustos. Dynamics of pseudo-radioactive chemical products via sampling theory. *Journal of Mathematical Chemistry*, 50(2):374–378, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-010-9788-x`.

Vigo-Aguiar:2012:CSM

[1930] Jesús Vigo-Aguiar, Ian Hamilton, and Stephen K. Gray. Computer science and mathematics for chemistry-related applications. *Journal of Mathematical Chemistry*, 50(2):379–380, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9964-7; http://link.springer.com/content/pdf/10.1007/s10910-011-9964-7.pdf`.

Canto:2012:DOG

[1931] B. Cantó, S. C. Cardona, C. Coll, J. Navarro-Laboulais, and E. Sánchez. Dynamic optimization of a gas-liquid reactor. *Journal of Mathematical Chemistry*, 50(2):381–393, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9941-1`.

Alonso-Sanchez:2012:DAC

[1932] T. Alonso-Sánchez, M. A. Rey-Ronco, M. P. Castro-García, and F. J. Carnero-Rodríguez. Design for an asymmetrical cyclic neutron activa-

tion process for determining fluorite grade in fluorspar concentrate. *Journal of Mathematical Chemistry*, 50(2):394–409, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9918-0`.

Alonso:2012:DPS

[1933] P. Alonso, F. Argüeso, R. Cortina, J. Ranilla, and A. M. Vidal. Detecting point sources in CMB maps using an efficient parallel algorithm. *Journal of Mathematical Chemistry*, 50(2):410–420, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9936-y`.

Strunk:2012:PSP

[1934] Timo Strunk, Moritz Wolf, and Wolfgang Wenzel. Peptide structure prediction using distributed volunteer computing networks. *Journal of Mathematical Chemistry*, 50(2):421–428, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9937-x`.

Fernandez:2012:NBL

[1935] José R. Fernández, María del Carmen Muñiz, and Cristina Núñez. Numerical behavior of a linear mixed kinetic-diffusion model for surfactant adsorption at the air-water interface. *Journal of Mathematical Chemistry*, 50(2):429–438, February 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9899-z`.

Cassam-Chenai:2012:GE

[1936] Patrick Cassam-Chenaï. Guest editorial. *Journal of Mathematical Chemistry*, 50(3):439, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9959-4; http://link.springer.com/content/pdf/10.1007/s10910-011-9959-4.pdf`.

Ebrahimi-Fard:2012:HLM

[1937] Kurusch Ebrahimi-Fard and José M. Gracia-Bondía. Harmonium as a laboratory for mathematical chemistry. *Journal of Mathematical Chemistry*, 50(3):440–454, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9822-7`.

Weiner:2012:GC

[1938] Brian Weiner. Generalized P, Q and G conditions. *Journal of Mathematical Chemistry*, 50(3):455–491, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9842-3`.

Valdemoro:2012:CPH

[1939] Carmela Valdemoro, Diego R. Alcoba, Ofelia B. Oña, Luis M. Tel, and Encarnación Pérez-Romero. Combining the G-particle-hole hypervirial equation and the Hermitian operator method to study electronic excitations and de-excitations. *Journal of Mathematical Chemistry*, 50 (3):492–509, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9810-y`.

Pestka:2012:GDC

[1940] Grzegorz Pestka, Mirosław Bylicki, and Jacek Karwowski. Geminals in Dirac–Coulomb Hamiltonian eigenvalue problem. *Journal of Mathematical Chemistry*, 50(3):510–533, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9823-6`.

Surjan:2012:SOG

[1941] Péter R. Surján, Ágnes Szabados, Péter Jeszenszki, and Tamás Zoboki. Strongly orthogonal geminals: size-extensive and variational reference states. *Journal of Mathematical Chemistry*, 50(3):534–551, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9849-9`.

Brouder:2012:NND

[1942] Christian Brouder and Frédéric Patras. Nonlocal, noncommutative diagrammatics and the linked cluster theorems. *Journal of Mathematical Chemistry*, 50(3):552–576, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9828-1`.

Marquardt:2012:NLA

[1943] Roberto Marquardt. Non linear adjustments with external conditions. *Journal of Mathematical Chemistry*, 50(3):577–587, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9819-2`.

Rist:2012:MCE

[1944] Claire Rist and Alexandre Faure. A Monte Carlo error estimator for the expansion of rigid-rotor potential energy surfaces. *Journal of Mathematical Chemistry*, 50(3):588–601, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9821-8`.

Bourquin:2012:NAT

[1945] Raoul Bourquin, Vasile Gradinaru, and George A. Hagedorn. Non-adiabatic transitions near avoided crossings: theory and numerics. *Journal of Mathematical Chemistry*, 50(3):602–619, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9827-2`.

Fermanian-Kammerer:2012:SSS

[1946] Clotilde Fermanian-Kammerer and Caroline Lasser. Single switch surface hopping for molecular quantum dynamics. *Journal of Mathematical Chemistry*, 50(3):620–635, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9816-5`.

Szalay:2012:PGB

[1947] Viktor Szalay, Tamás Szidarovszky, Gábor Czakó, and Attila G. Császár. A paradox of grid-based representation techniques: accurate eigenvalues from inaccurate matrix elements. *Journal of Mathematical Chemistry*, 50 (3):636–651, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9843-2`.

Cassam-Chenai:2012:FAQ

[1948] P. Cassam-Chenaï and A. Ilmane. Frequently asked questions on the mean field configuration interaction method. I — Distinguishable degrees of freedom. *Journal of Mathematical Chemistry*, 50(3):652–667, March 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9912-6`.

Tachibana:2012:GRS

[1949] Akitomo Tachibana. General relativistic symmetry of electron spin torque. *Journal of Mathematical Chemistry*, 50(4):669–688, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9943-z`.

Han:2012:FDA

[1950] Weimin Han, Joseph A. Eichholz, and Ge Wang. On a family of differential approximations of the radiative transfer equation. *Journal of Mathematical Chemistry*, 50(4):689–702, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9916-2`.

Irsai:2012:SSE

[1951] Izabella Irsai, Cornelia Majdik, Alexandru Lupan, and Radu Silaghi-Dumitrescu. Secondary structure elements in polylactic acid models. *Journal of Mathematical Chemistry*, 50(4):703–733, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9919-z`.

Carbo-Dorca:2012:SED

[1952] Ramon Carbó-Dorca. Scaled Euclidian distances: a general dissimilarity index with a suitably defined geometrical foundation. *Journal of Mathematical Chemistry*, 50(4):734–740, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9920-6`.

Carbo-Dorca:2012:SOT

[1953] Ramon Carbó-Dorca. Symmetrical overlap transformations of function basis sets: the LCAO MO and quantum similarity practical cases. *Journal of Mathematical Chemistry*, 50(4):741–751, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9921-5`.

Li:2012:IMM

[1954] Banghe Li, Bo Li, and Yuefeng Shen. An improved method to measure all rate constants in the simplest enzyme kinetics model. *Journal of Mathematical Chemistry*, 50(4):752–764, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9922-4`.

Bieniasz:2012:ASE

[1955] Lesław K. Bieniasz. Automatic simulation of electrochemical transients by the adaptive Huber method for Volterra integral equations involving kernel terms $\exp[-\alpha(t-\tau)]\mathrm{erex}\{[\beta(t-\tau)]^{1/2}\}$ and $\exp[-\alpha(t-\tau)]\mathrm{daw}\{[\beta(t\tau)]^{1/2}\}$. *Journal of Mathematical Chemistry*, 50(4):765–781, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9923-3`.

Alolyan:2012:NOM

[1956] Ibraheem Alolyan and T. E. Simos. New open modified trigonometrically-fitted Newton–Cotes type multilayer symplectic integrators for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 50(4):782–804, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9924-2`.

Gimre:2012:ADK

[1957] K. T. Gimre, R. V. Whiteley, Jr., and C. M. Guenther. The analytical determination of kinetic parameters for a bimolecular EC mechanism from chronoamperometric data. *Journal of Mathematical Chemistry*, 50 (4):805–818, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9925-1`.

Bhattacharjee:2012:BSQ

[1958] Shayak Bhattacharjee, D. S. Ray, and J. K. Bhattacharjee. Bohr–Sommerfeld quantisation and molecular potentials. *Journal of Mathematical Chemistry*, 50(4):819–832, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9926-0`.

Marmorino:2012:OTL

[1959] M. G. Marmorino, Abdullah Almayouf, Tyler Krause, and Doan Le. Optimization of the Temple lower bound. *Journal of Mathematical Chemistry*, 50(4):833–842, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9927-z`.

Mezey:2012:UEV

[1960] Paul G. Mezey. Unexpected expectation values for latent molecular properties. *Journal of Mathematical Chemistry*, 50(4):843–849, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9928-y`.

Demiralp:2012:PFDa

[1961] Metin Demiralp, Emre Demiralp, and Luis Hernandez-Garcia. A probabilistic foundation for dynamical systems: theoretical background and mathematical formulation. *Journal of Mathematical Chemistry*, 50(4): 850–869, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9929-x`.

Demiralp:2012:PFDb

[1962] Emre Demiralp, Metin Demiralp, and Luis Hernandez-Garcia. A probabilistic foundation for dynamical systems: phenomenological reasoning and principal characteristics of probabilistic evolution. *Journal of Mathematical Chemistry*, 50(4):870–880, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9930-4`.

Dong:2012:ESM

[1963] Shi-Hai Dong and M. Cruz-Irisson. Energy spectrum for a modified Rosen–Morse potential solved by proper quantization rule and its thermodynamic properties. *Journal of Mathematical Chemistry*, 50(4): 881–892, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9931-3`.

Pisanski:2012:FGT

[1964] Tomaz Pisanski and Alexandru T. Balaban. Flag graphs and their applications in mathematical chemistry for benzenoids. *Journal of Mathematical Chemistry*, 50(4):893–903, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9932-2`.

Karimi:2012:CGA

[1965] Sasan Karimi, Anthony Delgado, and Marty Lewinter. A combinatorial/geometric analysis of parallelogram-like benzenoids. *Journal of Mathematical Chemistry*, 50(4):904–913, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9933-1`.

March:2012:EMC

[1966] N. H. March, G. G. N. Angilella, and R. Pucci. Equation of motion of the correlated first-order density matrix for the ground-state of the Hookean atom with two electrons. *Journal of Mathematical Chemistry*, 50(4):914–919, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9934-0`.

Zhang:2012:PCB

[1967] Z. D. Zhang and N. H. March. Proposed connection between critical exponents and fractal dimensions in the Ising model. *Journal of Mathematical Chemistry*, 50(4):920–925, April 2012. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9935-z.

Mezey:2012:MFS

[1968] Paul G. Mezey. Molecular fragment shape variation index for functional groups and the holographic properties of electron density. *Journal of Mathematical Chemistry*, 50(4):926–933, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9938-9.

Simon:2012:FSV

[1969] Eva Simon and Paul G. Mezey. Fragment shape variation index for periodicity deficiency and gradual changes of internal coordinates along linear polymers. *Journal of Mathematical Chemistry*, 50(4):934–941, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9939-8.

Antal:2012:MFS

[1970] Zoltan Antal and Paul G. Mezey. Molecular fragment shape variation index applied to intramolecular interaction studies. *Journal of Mathematical Chemistry*, 50(4):942–948, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9940-2.

Arteca:2012:CQM

[1971] Gustavo A. Arteca, Josep M. Aulló, and O. Tapia. Constructing quantum mechanical models starting from diabatic schemes: Quantum states for simulations bond break/formation — I. Feshbach-like quantum states and electronuclear wave functions. *Journal of Mathematical Chemistry*, 50(4):949–970, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9942-0.

Arda:2012:ESS

[1972] Altug Arda and Ramazan Sever. Exact solutions of the Schrödinger equation via Laplace transform approach: pseudoharmonic potential and Mie-type potentials. *Journal of Mathematical Chemistry*, 50(4):971–980, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9944-y.

Carbo-Dorca:2012:NAS

[1973] Ramon Carbó-Dorca and Emili Besalú. On the nature of atomic shell approximation (ASA) electrostatic molecular potentials (EMP). *Journal of Mathematical Chemistry*, 50(4):981–988, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9945-x`.

Smith:2012:GDS

[1974] Hal L. Smith. Global dynamics of the smallest chemical reaction system with Hopf bifurcation. *Journal of Mathematical Chemistry*, 50 (4):989–995, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9946-9`.

Lu:2012:MVC

[1975] Dan Lu, Pan-Pan Zhou, and Wen-Yuan Qiu. Models of virus capsids containing 72 pentameric capsomeres. *Journal of Mathematical Chemistry*, 50(4):996–1002, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9947-8`.

Petrov:2012:CRR

[1976] Vesselin Petrov and Fernando Pina. Complete resolution of the reaction rates of flavylium networks. The role played by 2-phenyl-2H-chromen-4-ol and the hydroxyl attack to the quinoidal base. *Journal of Mathematical Chemistry*, 50(4):1003–1019, April 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9948-7`.

Strekalov:2012:LPS

[1977] M. L. Strekalov. Laguerre polynomial solutions to master equation for vibrational energy relaxation in gases. *Journal of Mathematical Chemistry*, 50(5):1021–1030, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9951-z`.

Chou:2012:CZZ

[1978] Chien-Pin Chou and Henryk A. Witek. Comment on "Zhang–Zhang polynomials of cyclo-polyphenacenes" by Q. Guo, H. Deng, and D. Chen. *Journal of Mathematical Chemistry*, 50(5):1031–1033, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9969-2`. See [1507].

Bucknum:2012:DCN

[1979] Michael J. Bucknum and Eduardo A. Castro. On the n-diamond and i-carbon nanocrystalline forms. *Journal of Mathematical Chemistry*, 50 (5):1034–1038, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9954-9`.

Oyewumi:2012:ESS

[1980] K. J. Oyewumi and K. D. Sen. Exact solutions of the Schrödinger equation for the pseudoharmonic potential: an application to some diatomic molecules. *Journal of Mathematical Chemistry*, 50(5):1039–1059, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9967-4`.

Sultan:2012:CSP

[1981] S. R. Sultan, W. J. N. Fernando, and Suhairi A. Sata. Coupled single-particle growth and kinetics modeling for styrene polymerization over silica-supported metallocene catalyst. *Journal of Mathematical Chemistry*, 50(5):1060–1078, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9949-6`.

Aptekarev:2012:REI

[1982] A. I. Aptekarev, J. S. Dehesa, P. Sánchez-Moreno, and D. N. Tulyakov. Rényi entropy of the infinite well potential in momentum space and Dirichlet-like trigonometric functionals. *Journal of Mathematical Chemistry*, 50(5):1079–1090, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9950-0`.

Lim:2012:PSP

[1983] Teik-Cheng Lim. A power series potential energy function with adjustable index. *Journal of Mathematical Chemistry*, 50(5):1091–1099, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9952-y`.

Bairamov:2012:SES

[1984] Elgiz Bairamov, Rukiye Özturk Mert, and Zameddin Ismailov. Selfadjoint extensions of a singular differential operator. *Journal of Mathematical Chemistry*, 50(5):1100–1110, May 2012. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9953-x.

Mincheva:2012:ONM

[1985] Maya Mincheva. Oscillations in non-mass action kinetics models of biochemical reaction networks arising from pairs of subnetworks. *Journal of Mathematical Chemistry*, 50(5):1111–1125, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9955-8.

Han:2012:SII

[1986] Weimin Han, Kendall Atkinson, and Hao Zheng. Some integral identities for spherical harmonics in an arbitrary dimension. *Journal of Mathematical Chemistry*, 50(5):1126–1135, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9956-7.

DellAcqua:2012:PSM

[1987] Guido Dell'Acqua and Alberto Maria Bersani. A perturbation solution of Michaelis–Menten kinetics in a "total" framework. *Journal of Mathematical Chemistry*, 50(5):1136–1148, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9957-6.

Strekalov:2012:USR

[1988] M. L. Strekalov. A uniform semiclassical representation of transition probabilities derived from factorization formulas. *Journal of Mathematical Chemistry*, 50(5):1149–1160, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9958-5.

Carbo-Dorca:2012:COS

[1989] Ramon Carbó-Dorca and Emili Besalú. Centroid origin shift of quantum object sets and molecular point clouds description and element comparisons. *Journal of Mathematical Chemistry*, 50(5):1161–1178, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9960-y.

Nagy:2012:MRD

[1990] Ilona Nagy and János Tóth. Microscopic reversibility or detailed balance in ion channel models. *Journal of Mathematical Chemistry*, 50 (5):1179–1199, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-011-9961-x.

Rajasingh:2012:PHN

[1991] Indra Rajasingh, Albert Muthumalai, R. Bharati, and A. S. Shanthi. Packing in honeycomb networks. *Journal of Mathematical Chemistry*, 50 (5):1200–1209, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9962-9`.

Arimoto:2012:MMM

[1992] Shigeru Arimoto. Multidimensional magic mountains and matrix art for the generalized repeat space theory. *Journal of Mathematical Chemistry*, 50(5):1210–1223, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9963-8`.

Simos:2012:HOC

[1993] T. E. Simos. High order closed Newton–Cotes exponentially and trigonometrically fitted formulae as multilayer symplectic integrators and their application to the radial Schrödinger equation. *Journal of Mathematical Chemistry*, 50(5):1224–1261, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9965-6`.

Hutem:2012:NES

[1994] Artit Hutem and Sutee Boonchui. Numerical evaluation of second and third virial coefficients of some inert gases via classical cluster expansion. *Journal of Mathematical Chemistry*, 50(5):1262–1276, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9966-5`.

Indira:2012:AEN

[1995] K. Indira and L. Rajendran. Analytical expression of non steady-state concentration for the CE mechanism at a planar electrode. *Journal of Mathematical Chemistry*, 50(5):1277–1288, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9968-3`.

Lee:2012:GFI

[1996] Richard K. F. Lee and James M. Hill. General formulae for interacting spherical nanoparticles and fullerenes. *Journal of Mathematical Chemistry*, 50(5):1289–1303, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9970-9`.

Wu:2012:LYC

[1997] Xinxing Wu and Peiyong Zhu. Li–Yorke chaos in a coupled lattice system related with Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 50(5):1304–1308, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9971-8`.

Xing:2012:SFS

[1998] Shengkai Xing, Yun Li, Xuezhuang Zhao, Zunsheng Cai, Zhenfeng Shang, Xiufang Xu, Ruifang Li, and Guichang Wang. Symmetries and fuzzy symmetries of graphene molecules. *Journal of Mathematical Chemistry*, 50(5):1309–1332, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9972-7`.

PonRani:2012:MMS

[1999] V. Margret PonRani and L. Rajendran. Mathematical modelling of steady-state concentration in immobilized glucose isomerase of packed-bed reactors. *Journal of Mathematical Chemistry*, 50(5):1333–1346, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-011-9973-6`.

Barany:2012:EDM

[2000] Mate Barany, Botond Bertok, Csanad Imreh, L. T. Fan, and Ferenc Friedler. On the equivalence of direct mechanisms and structurally minimal pathways. *Journal of Mathematical Chemistry*, 50(5):1347–1361, May 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9974-0`.

Estrada:2012:RCD

[2001] Ernesto Estrada. Returnability as a criterion of disequilibrium in atmospheric reactions networks. *Journal of Mathematical Chemistry*, 50 (6):1363–1372, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9977-x`.

Goeke:2012:NKS

[2002] Alexandra Goeke, Christian Schilli, Sebastian Walcher, and Eva Zerz. A note on the kinetics of suicide substrates. *Journal of Mathematical Chemistry*, 50(6):1373–1377, June 2012. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9979-8`.

Cioslowski:2012:EEP

[2003] Jerzy Cioslowski and Joanna Albin. Electrostatic energy of polygonal charge distributions. *Journal of Mathematical Chemistry*, 50(6): 1378–1385, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9975-z`.

Cheng:2012:BIP

[2004] Xiao-Sheng Cheng, Xiaoyan Jiang, and Huawei Dai. The braid index of polyhedral links. *Journal of Mathematical Chemistry*, 50(6):1386–1397, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9976-y`.

Bhattacharjee:2012:LPT

[2005] Shayak Bhattacharjee and J. K. Bhattacharjee. Lindstedt–Poincaré technique applied to molecular potentials. *Journal of Mathematical Chemistry*, 50(6):1398–1410, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9978-9`.

Angerer:2012:ESM

[2006] Wolfgang P. Angerer and Adolfo Zamora. Eigenvalues of a statistical mechanics matrix. *Journal of Mathematical Chemistry*, 50(6):1411–1419, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9980-2`.

VanGorder:2012:SEN

[2007] Robert A. Van Gorder. Schrödinger equations on $\mathbf{r}^3 \times \Updownarrow$ with non-separable potential. *Journal of Mathematical Chemistry*, 50(6):1420–1436, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9981-1`.

Nalewajski:2012:BSD

[2008] Roman F. Nalewajski, Dariusz Szczepanik, and Janusz Mrozek. Basis set dependence of molecular information channels and their entropic bond descriptors. *Journal of Mathematical Chemistry*, 50(6):1437–1457,

June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-9982-0; http://link.springer.com/content/pdf/10.1007/s10910-012-9982-0.pdf.

Hubler:2012:MDL

[2009] Shane L. Hubler and Gheorghe Craciun. Mass distributions of linear chain polymers. *Journal of Mathematical Chemistry*, 50(6):1458–1483, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-9983-z.

Arda:2012:NCP

[2010] Altug Arda and Ramazan Sever. Non-central potentials, exact solutions and Laplace transform approach. *Journal of Mathematical Chemistry*, 50 (6):1484–1494, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-9984-y.

Goeke:2012:CQS

[2011] Alexandra Goeke, Christian Schilli, Sebastian Walcher, and Eva Zerz. Computing quasi-steady state reductions. *Journal of Mathematical Chemistry*, 50(6):1495–1513, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-9985-x.

Barabas:2012:SGR

[2012] Béla Barabás and Ottilia Fülöp. Star graph representations of chiral objects in graph theory. *Journal of Mathematical Chemistry*, 50(6): 1514–1520, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-9986-9.

Pesonen:2012:NMA

[2013] Janne Pesonen, Krister O. E. Henriksson, Jose Ramon López-Blanco, and Pablo Chacón. Normal mode analysis of molecular motions in curvilinear coordinates on a non-Eckart body-frame: an application to protein torsion dynamics. *Journal of Mathematical Chemistry*, 50(6):1521–1549, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-9987-8.

Lee:2012:AAS

[2014] Chang Hyeong Lee and Pilwon Kim. An analytical approach to solutions of master equations for stochastic nonlinear reactions. *Journal of Mathematical Chemistry*, 50(6):1550–1569, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9988-7`.

Bancewicz:2012:EHI

[2015] Tadeusz Bancewicz. Excess hyperpolarizabilities: the irreducible tensor approach. *Journal of Mathematical Chemistry*, 50(6):1570–1581, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9990-0; http://link.springer.com/content/pdf/10.1007/s10910-012-9990-0.pdf`.

Boonchui:2012:ESEa

[2016] Sutee Boonchui and Artit Hutem. Excited-state energy eigenvalue and wave-function evaluation of the Gaussian symmetric double-well potential problem via numerical shooting method 1. *Journal of Mathematical Chemistry*, 50(6):1582–1597, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9996-7`.

Garcia-Sevilla:2012:LCSa

[2017] Francisco Garcia-Sevilla, Manuela Garcia-Moreno, Milagros Molina-Alarcon, María J. Garcia-Meseguer, José M. Villalba, Enrique Arribas, and Ramón Varon. Linear compartmental systems. I. Kinetic analysis and derivation of their optimized symbolic equations. *Journal of Mathematical Chemistry*, 50(6):1598–1624, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9991-z`.

Garcia-Sevilla:2012:LCSb

[2018] Francisco Garcia-Sevilla, Manuela Garcia-Moreno, Milagros Molina-Alarcon, María J. Garcia-Meseguer, José M. Villalba, Enrique Arribas, and Ramón Varon. Linear compartmental systems: II — a software to obtain the symbolic kinetic equations. *Journal of Mathematical Chemistry*, 50(6):1625–1648, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9992-y`.

Kipriyanov:2012:IFI

[2019] Alexander A. Kipriyanov, Alexander A. Kadetov, Alexey A. Kipriyanov, and Alexander B. Doktorov. Influence of the force interaction on accumulation of macroscopic correlations in elementary reaction $A + B \to C$. *Journal of Mathematical Chemistry*, 50(6):1649–1692, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9993-x`.

Deng:2012:ETC

[2020] Kecai Deng, Jianguo Qian, and Fuji Zhang. Enumerating the total colorings of a polyhedron and application to polyhedral links. *Journal of Mathematical Chemistry*, 50(6):1693–1705, June 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9994-9`.

Glasser:2012:MPH

[2021] M. L. Glasser and I. Nagy. Moments of powers of the Hulthén density. *Journal of Mathematical Chemistry*, 50(7):1707–1710, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0014-x`.

Tunga:2012:MDM

[2022] M. Alper Tunga and Metin Demiralp. Multivariate data modelling through piecewise generalized HDMR method. *Journal of Mathematical Chemistry*, 50(7):1711–1726, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0001-2`.

Torres:2012:PSP

[2023] Emilio Martínez Torres. Partition of symmetric powers of G-sets into orbits: application to the enumeration of force constants. *Journal of Mathematical Chemistry*, 50(7):1727–1735, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0002-1`.

Monovasilis:2012:PFS

[2024] Th. Monovasilis. Phase fitted symplectic partitioned Runge–Kutta methods for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 50(7):1736–1746, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0003-0`.

Li:2012:DMR

[2025] Genyuan Li, Roberto Rey de Castro, and Herschel Rabitz. D-MORPH regression for modeling with fewer unknown parameters than observation data. *Journal of Mathematical Chemistry*, 50(7):1747–1764, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0004-z`.

Izmailov:2012:SAM

[2026] Sofia Izmailov, XiaoJiang Feng, Genyuan Li, and Herschel Rabitz. A scalable algorithm for molecular property estimation in high dimensional scaffold-based libraries. *Journal of Mathematical Chemistry*, 50(7): 1765–1790, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0005-y`.

Fujita:2012:STBa

[2027] Shinsaku Fujita. Stereoisograms of trigonal bipyramidal compounds: I. Chirality and RS-stereogenicity free from the conventional "chirality" and "stereogenicity". *Journal of Mathematical Chemistry*, 50(7): 1791–1814, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0006-x`.

Fujita:2012:STBb

[2028] Shinsaku Fujita. Stereoisograms of trigonal bipyramidal compounds: II. RS-stereogenicity/RS-stereoisomerism versus stereogenicity/stereoisomerism, leading to a revised interpretation of Berry's pseudorotation. *Journal of Mathematical Chemistry*, 50(7):1815–1860, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0007-9`.

Alolyan:2012:NHT

[2029] Ibraheem Alolyan and T. E. Simos. A new hybrid two-step method with vanished phase-lag and its first and second derivatives for the numerical solution of the Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 50(7):1861–1881, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0008-8`.

Molina-Espiritu:2012:ITC

[2030] Moyocoyani Molina-Espíritu, Rodolfo O. Esquivel, Juan Carlos Angulo, Juan Antolín, and Jesús S. Dehesa. Information-theoretical complexity

for the hydrogenic identity S_N2 exchange reaction. *Journal of Mathematical Chemistry*, 50(7):1882–1900, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0009-7`.

Rogerson:2012:SLS

[2031] Parker Rogerson and Gustavo A. Arteca. Scaling laws in simple and complex proteins: size scaling effects associated with domain number and folding class. *Journal of Mathematical Chemistry*, 50(7):1901–1919, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0010-1`.

Arda:2012:AAS

[2032] Altug Arda and Ramazan Sever. Approximate analytical solutions of a two-term diatomic molecular potential with centrifugal barrier. *Journal of Mathematical Chemistry*, 50(7):1920–1930, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0011-0`.

Simpao:2012:HHO

[2033] Valentino A. Simpao. HOA (Heaviside Operational Ansatz) revisited: recent remarks on novel exact solution methodologies in wavefunction analysis. *Journal of Mathematical Chemistry*, 50(7):1931–1972, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0012-z`. See [1407].

Akcay:2012:ASS

[2034] Huseyin Akcay and Ramazan Sever. Analytical solutions of Schrödinger equation for the diatomic molecular potentials with any angular momentum. *Journal of Mathematical Chemistry*, 50(7):1973–1987, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0013-y`.

Huang-Fu:2012:SSE

[2035] Guo-Qing Huang-Fu and Min-Cang Zhang. Solutions of the Schrödinger equation in the tridiagonal representation with the noncentral electric dipole plus a novel angle-dependent component. *Journal of Mathematical Chemistry*, 50(7):1988–2000, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0015-9`.

Puida:2012:MEC

[2036] Mantas Puida, Albertas Malinauskas, and Feliksas Ivanauskas. Modeling of electrocatalysis at chemically modified electrodes: a combination of second-order and Michaelis-type chemical kinetics. *Journal of Mathematical Chemistry*, 50(7):2001–2011, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0016-8`.

Rosenfeld:2012:EPI

[2037] Vladimir R. Rosenfeld, Douglas J. Klein, and Josep M. Oliva. Enumeration of polycarborane isomers: especially dicarboranes. *Journal of Mathematical Chemistry*, 50(7):2012–2022, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0017-7`.

Ozay:2012:CSS

[2038] Evrim Korkmaz Özay and Metin Demiralp. Combined small scale high dimensional model representation. *Journal of Mathematical Chemistry*, 50(7):2023–2042, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0018-6`.

LeDell:2012:CNP

[2039] Erin LeDell, Prabhat, Dmitry Yu. Zubarev, Brian Austin, and William A. Lester, Jr. Classification of nodal pockets in many-electron wave functions via machine learning. *Journal of Mathematical Chemistry*, 50(7):2043–2050, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0019-5`.

Killingbeck:2012:CPQ

[2040] J. P. Killingbeck and A. Lakhlifi. Calculating probabilities without quadrature. *Journal of Mathematical Chemistry*, 50(7):2051–2060, August 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0020-z`.

Quapp:2012:TCR

[2041] Wolfgang Quapp and Josep Maria Bofill. Topography of cyclopropyl radical ring opening to allyl radical on the CASSCF(3,3) surface: valley-ridge inflection points by Newton trajectories. *Journal of Mathematical Chemistry*, 50(8):2061–2085, September 2012. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9995-8`.

Hutem:2012:ECE

[2042] Artit Hutem and Sutee Boonchui. Evaluation of Coulomb and exchange integrals for higher excited states of helium atom by using spherical harmonics series. *Journal of Mathematical Chemistry*, 50(8):2086–2102, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9997-6`.

Boonchui:2012:ESEb

[2043] Sutee Boonchui and Artit Hutem. Excited-state energy eigenvalue and wave-function evaluation of the Gaussian asymmetric double-well potential problem via numerical shooting method 2. *Journal of Mathematical Chemistry*, 50(8):2103–2119, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9998-5`.

Krukle-Berzina:2012:NMS

[2044] Kristine Krukle-Berzina, Andris Actins, and Agris Berzins. A new methodology for the simulation of solid state phase transition kinetics by combination of nucleation and nuclei growth processes. *Journal of Mathematical Chemistry*, 50(8):2120–2129, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-9999-4`.

Gubernov:2012:PCW

[2045] V. V. Gubernov, J. J. Sharples, H. S. Sidhu, A. C. McIntosh, and J. Brindley. Properties of combustion waves in the model with competitive exo- and endothermic reactions. *Journal of Mathematical Chemistry*, 50(8):2130–2140, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0021-y`.

Ponomarev:2012:MNH

[2046] Denis Ponomarev, Elisabeth Rodier, Martial Sauceau, Clémence Nikitine, Vadim Mizonov, and Jacques Fages. Modelling non-homogeneous flow and residence time distribution in a single-screw extruder by means of Markov chains. *Journal of Mathematical Chemistry*, 50(8):2141–2154, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0022-x`.

Massaccesi:2012:SAF

[2047] Gustavo E. Massaccesi, Diego R. Alcoba, and Ofelia B. Oña. Symmetry-adapted formulation of the G-particle-hole hypervirial equation method. *Journal of Mathematical Chemistry*, 50(8):2155–2167, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0023-9`.

Fujita:2012:IPPa

[2048] Shinsaku Fujita. Importance of the proligand-promolecule model in stereochemistry. II. The stereoisogram approach to stereoisomeric features of prismane derivatives. *Journal of Mathematical Chemistry*, 50(8):2168–2201, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0024-8`.

Fujita:2012:IPPb

[2049] Shinsaku Fujita. Importance of the proligand-promolecule model in stereochemistry. I. The unit-subduced-cycle-index (USCI) approach to geometric features of prismane derivatives. *Journal of Mathematical Chemistry*, 50(8):2202–2222, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0025-7`.

Tunga:2012:HHM

[2050] Burcu Tunga and Metin Demiralp. Hybrid HDMR method with an optimized hybridity parameter in multivariate function representation. *Journal of Mathematical Chemistry*, 50(8):2223–2238, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0026-6`.

Zhang:2012:GAC

[2051] Tonghua Zhang. Global analysis of continuous flow bioreactor and membrane reactor models with death and maintenance. *Journal of Mathematical Chemistry*, 50(8):2239–2247, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0027-5`.

Zhao:2012:MTG

[2052] Xuezhuang Zhao, Shengkai Xing, Yun Li, Zunsheng Cai, Yinming Pan, Zhenfeng Shang, Guichang Wang, Xiufang Xu, and Ruifang Li. Molecular torus group. *Journal of Mathematical Chemistry*, 50(8):2248–2271, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0028-4.

Fowler:2012:FSC

[2053] Patrick W. Fowler, Mohammadreza Jooyandeh, and Gunnar Brinkmann. Face-spiral codes in cubic polyhedral graphs with face sizes no larger than 6. *Journal of Mathematical Chemistry*, 50(8):2272–2280, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0029-3.

Bucknum:2012:I

[2054] Michael J. Bucknum, Eduardo A. Castro, and Bin Wen. Isoglitter. *Journal of Mathematical Chemistry*, 50(8):2281–2290, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0030-x.

Mackevicius:2012:CLC

[2055] Mazvydas Mackevicius, Feliksas Ivanauskas, Aivaras Kareiva, and Darius Jasaitis. A closer look at the computer modeling and sintering optimization in the preparation of YAG. *Journal of Mathematical Chemistry*, 50(8):2291–2302, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0031-9.

Mukherjee:2012:NSD

[2056] Neetik Mukherjee. New state dependent uncertainty principle and design of objective function for optimisation: utility of kinetic and potential energy uncertainties. *Journal of Mathematical Chemistry*, 50(8):2303–2316, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0032-8.

Pourgholi:2012:AHB

[2057] R. Pourgholi, N. Tavallaie, and S. Foadian. Applications of Haar basis method for solving some ill-posed inverse problems. *Journal of Mathematical Chemistry*, 50(8):2317–2337, September 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0036-4.

Carbo-Dorca:2012:QSM

[2058] Ramon Carbó-Dorca. Quantum similarity matrices column set as holograms of DF molecular point clouds. *Journal of Mathematical Chem-*

istry, 50(9):2339–2341, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0034-6`.

Hudelson:2012:DPA

[2059] Matthew Hudelson, Barbara Logan Mooney, and Aurora E. Clark. Determining polyhedral arrangements of atoms using PageRank. *Journal of Mathematical Chemistry*, 50(9):2342–2350, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0033-7`.

Alolyan:2012:NHO

[2060] Ibraheem Alolyan and T. E. Simos. A new high order two-step method with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 50(9):2351–2373, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0035-5`.

Wei:2012:TSS

[2061] Meihua Wei, Jianhua Wu, and Gaihui Guo. Turing structures and stability for the 1-D Lengyel–Epstein system. *Journal of Mathematical Chemistry*, 50(9):2374–2396, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0037-3; http://www.springerlink.com/content/4865417834u11n37/`.

Marmorino:2012:LBG

[2062] M. G. Marmorino, Abdullah Almayouf, Tyler Krause, and Doan Le. Lower bound to the ground-state expectation value of a positive unbounded operator using related bounded operators. *Journal of Mathematical Chemistry*, 50(9):2397–2407, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0038-2`.

Fowler:2012:CPA

[2063] Patrick W. Fowler, Wendy Myrvold, and William H. Bird. Counterexamples to a proposed algorithm for Fries structures of benzenoids. *Journal of Mathematical Chemistry*, 50(9):2408–2426, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0039-1`.

Kaushik:2012:ASN

[2064] Aditya Kaushik and Ved Prakash Kaushik. Analytic solution of nonlinear singularly perturbed initial value problems through iteration. *Journal of Mathematical Chemistry*, 50(9):2427–2438, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0040-8`.

Wu:2012:PMD

[2065] Xinxing Wu and Peiyong Zhu. The principal measure and distributional (p, q)-chaos of a coupled lattice system related with Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 50(9):2439–2445, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0041-7`.

Hubler:2012:CCC

[2066] Shane L. Hubler and Gheorghe Craciun. Counting chemical compositions using Ehrhart quasi-polynomials. *Journal of Mathematical Chemistry*, 50(9):2446–2470, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0042-6`.

Kuzmin:2012:MMH

[2067] R. N. Kuzmin, D. S. Maximov, N. P. Savenkova, and A. V. Shobukhov. Mathematical modeling of hysteresis in porous electrodes. *Journal of Mathematical Chemistry*, 50(9):2471–2477, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0043-5`.

Alcoba:2012:DIG

[2068] Diego R. Alcoba, Ofelia B. Oña, Carmela Valdemoro, Luis M. Tel, and Gustavo E. Massaccesi. Drawing information from the ground state G-particle-hole matrix to study electronic excited states. *Journal of Mathematical Chemistry*, 50(9):2478–2491, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0044-4`.

Fusi:2012:DCC

[2069] Lorenzo Fusi, Alessandro Monti, and Mario Primicerio. Determining calcium carbonate neutralization kinetics from experimental laboratory data. *Journal of Mathematical Chemistry*, 50(9):2492–2511, October

2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0045-3.

Alshehri:2012:IDS

[2070] Mansoor H. Alshehri, Barry J. Cox, and James M. Hill. Interaction of double-stranded DNA inside single-walled carbon nanotubes. *Journal of Mathematical Chemistry*, 50(9):2512–2526, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0046-2.

Belkic:2012:MAS

[2071] Dzevad Belkić and Karen Belkić. A meta-analysis of studies using MR spectroscopy for evaluating suspicious lesions after radiation therapy of primary brain tumors. *Journal of Mathematical Chemistry*, 50(9):2527–2557, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0047-1.

Belkic:2012:MRS

[2072] Dzevad Belkić and Karen Belkić. Magnetic resonance spectroscopy with high-resolution and exact quantification in the presence of noise for improving ovarian cancer detection. *Journal of Mathematical Chemistry*, 50(9):2558–2576, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0049-z.

Milani:2012:DCF

[2073] G. Milani and F. Milani. Direct and closed form analytical model for the prediction of reaction kinetic of EPDM accelerated sulphur vulcanization. *Journal of Mathematical Chemistry*, 50(9):2577–2605, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0048-0.

Arimoto:2012:RST

[2074] Shigeru Arimoto, Mark Spivakovsky, Massoud Amini, Eiji Yoshida, Masaaki Yokotani, and Tokio Yamabe. Repeat space theory applied to carbon nanotubes and related molecular networks. III. *Journal of Mathematical Chemistry*, 50(9):2606–2622, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0050-6.

Fackeldey:2012:CGM

[2075] Konstantin Fackeldey, Martina Klimm, and Marcus Weber. A coarse graining method for the dimension reduction of the state space of biomolecules. *Journal of Mathematical Chemistry*, 50(9):2623–2635, October 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0051-5`.

Shan:2012:PCC

[2076] Hai-Ying Shan and Jia-Yu Shao. The proof of a conjecture on the comparison of the energies of trees. *Journal of Mathematical Chemistry*, 50(10):2637–2647, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0052-4`.

Killingbeck:2012:SHS

[2077] John P. Killingbeck and Alain Grosjean. A simple Hill-series approach to the linear potential. *Journal of Mathematical Chemistry*, 50(10):2648–2658, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0053-3`.

Zhang:2012:TTS

[2078] Min-Cang Zhang. Tridiagonal treatment for the Schrödinger equation with a noncentral electric dipole ring-shaped potential. *Journal of Mathematical Chemistry*, 50(10):2659–2670, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0055-1`.

Pasca:2012:QAA

[2079] Daniel Pasca and Cláudia Valls. Qualitative analysis of the anisotropic two-body problem with generalized Lennard-Jones potential. *Journal of Mathematical Chemistry*, 50(10):2671–2688, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0057-z`.

Orel:2012:CPM

[2080] Rok Orel and Milan Randić. On characterizing proteomics maps by using weighted Voronoi maps. *Journal of Mathematical Chemistry*, 50(10):2689–2702, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0058-y`.

Rodriguez:2012:BCF

[2081] Alex Rodriguez, M. Santos Tomas, and Jaime Rubio-Martinez. A benchmark calculation for the fuzzy c-means clustering algorithm: initial memberships. *Journal of Mathematical Chemistry*, 50(10):2703–2715, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0059-x`.

Buyukasik:2012:ESM

[2082] Sirin A. Büyükasik and Oktay K. Pashaev. Exactly solvable Madelung fluid and complex Burgers equations: a quantum Sturm–Liouville connection. *Journal of Mathematical Chemistry*, 50(10):2716–2745, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0060-4`.

Zhou:2012:HKT

[2083] Aihui Zhou. Hohenberg–Kohn theorem for Coulomb type systems and its generalization. *Journal of Mathematical Chemistry*, 50(10):2746–2754, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0061-3`.

Randic:2012:ECF

[2084] Milan Randić, Marjana Nović, and Dejan Plavsić. π-electron currents in fixed π-sextet aromatic benzenoids. *Journal of Mathematical Chemistry*, 50(10):2755–2774, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0062-2`.

Hariharan:2012:WMF

[2085] G. Hariharan, V. Ponnusami, and R. Srikanth. Wavelet method to film-pore diffusion model for methylene blue adsorption onto plant leaf powders. *Journal of Mathematical Chemistry*, 50(10):2775–2785, November 2012. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0063-1`.

Bhattacharyya:2013:MEU

[2086] Kamal Bhattacharyya and Karabi Halder. A mixed-entropic uncertainty relation. *Journal of Mathematical Chemistry*, 51(1):1–6, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0068-9`.

Nalewajski:2013:ITM

[2087] Roman F. Nalewajski. Information-theoretic multiplicities of chemical bond in Shull's model of H_2. *Journal of Mathematical Chemistry*, 51 (1):7–20, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0054-2; http://link.springer.com/content/pdf/10.1007/s10910-012-0054-2.pdf`.

Rosenfeld:2013:ESIa

[2088] Vladimir R. Rosenfeld and Douglas J. Klein. Enumeration of substitutional isomers with restrictive mutual positions of ligands: I. Overall counts. *Journal of Mathematical Chemistry*, 51(1):21–37, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0056-0`.

Demiralp:2013:CLRa

[2089] Metin Demiralp and Emre Demiralp. A contemporary linear representation theory for ordinary differential equations: multilinear algebra in folded arrays (folarrs) perspective and its use in multidimensional case. *Journal of Mathematical Chemistry*, 51(1):38–57, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0064-0`.

Demiralp:2013:CLRb

[2090] Metin Demiralp and Emre Demiralp. A contemporary linear representation theory for ordinary differential equations: probabilistic evolutions and related approximants for unidimensional autonomous systems. *Journal of Mathematical Chemistry*, 51(1):58–72, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0070-2`.

Lebedev:2013:SPR

[2091] A. V. Lebedev, M. V. Okun, V. A. Chorkov, P. M. Tokar, and M. Strelkova. Systematic procedure for reduction of kinetic mechanisms of complex chemical processes and its software implementation. *Journal of Mathematical Chemistry*, 51(1):73–107, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0065-z`.

Strekalov:2013:CET

[2092] M. L. Strekalov. Collisional energy transfer with statistical energy exchange: an analytical solution in the statistical limit. *Journal of Mathematical Chemistry*, 51(1):108–116, January 2013. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0066-y.

VanAlsenoy:2013:PIS

[2093] C. Van Alsenoy and N. H. March. Positive ions of SiH_4: Jahn–Teller-like distortions for SiH_4^+ and eventually molecular collapse on further ionisation. *Journal of Mathematical Chemistry*, 51(1):117–124, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://hdl.handle.net/10067/1059350151162165141; http://link.springer.com/article/10.1007/s10910-012-0067-x.

Morales-Bayuelo:2013:TMQ

[2094] Alejandro Morales-Bayuelo and Ricardo Vivas-Reyes. Topological model to quantify the global reactivity indexes as local in Diels–Alder reactions, using density function theory (DFT) and local quantum similarity (LQS). *Journal of Mathematical Chemistry*, 51(1):125–143, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0069-8.

Bispo:2013:SEC

[2095] Jose Ailton Conceicao Bispo, Carlos Francisco Sampaio Bonafe, Maria Gabriela Bello Koblitz, Carlos Geilson Santana Silva, and Ancelmo Rabelo de Souza. Substrate and enzyme concentration dependence of the Henri–Michaelis–Menten model probed by numerical simulation. *Journal of Mathematical Chemistry*, 51(1):144–152, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0071-1.

Joshi:2013:AMC

[2096] Badal Joshi and Anne Shiu. Atoms of multistationarity in chemical reaction networks. *Journal of Mathematical Chemistry*, 51(1):153–178, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0072-0.

Corzo:2013:MLD

[2097] H. H. Corzo, E. Castaño, H. G. Laguna, and R. P. Sagar. Measuring localization-delocalization phenomena in a quantum corral. *Journal of Mathematical Chemistry*, 51(1):179–193, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0073-z.

Simos:2013:NHO

[2098] T. E. Simos. New high order multiderivative explicit four-step methods with vanished phase-lag and its derivatives for the approximate solution of the Schrödinger equation. Part I: Construction and theoretical analysis. *Journal of Mathematical Chemistry*, 51(1):194–226, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0074-y`.

Hamzavi:2013:EES

[2099] M. Hamzavi, S. M. Ikhdair, and K.-E. Thylwe. Equivalence of the empirical shifted Deng–Fan oscillator potential for diatomic molecules. *Journal of Mathematical Chemistry*, 51(1):227–238, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0075-x`.

Rosenfeld:2013:ESIb

[2100] Vladimir R. Rosenfeld and Douglas J. Klein. Enumeration of substitutional isomers with restrictive mutual positions of ligands. II. Counts with restrictions on (sub)symmetry. *Journal of Mathematical Chemistry*, 51 (1):239–264, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0076-9`.

Castro:2013:TPS

[2101] L. B. Castro and A. S. de Castro. Trapping of a particle in a short-range harmonic potential well. *Journal of Mathematical Chemistry*, 51 (1):265–277, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0077-8`.

Phan:2013:TPT

[2102] Anh D. Phan, Lilia M. Woods, and N. A. Viet. Temperature phase transition model for the DNA–CNTs-based nanotweezers. *Journal of Mathematical Chemistry*, 51(1):278–288, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0082-y`.

Carbo-Dorca:2013:MAL

[2103] Ramon Carbó-Dorca. Mathematical aspects of the LCAO MO first order density function (5): centroid shifting of MO shape functions basis set, properties and applications. *Journal of Mathematical Chemistry*, 51(1): 289–296, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0083-x.

Nalewajski:2013:ERT

[2104] Roman F. Nalewajski. Entropic representation in the theory of molecular electronic structure. *Journal of Mathematical Chemistry*, 51(1): 297–315, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0084-9; http://link.springer.com/content/pdf/10.1007/s10910-012-0084-9.pdf.

Lee:2013:NCM

[2105] Chang Hyeong Lee, Jaemin Shin, and Junseok Kim. A numerical characteristic method for probability generating functions on stochastic first-order reaction networks. *Journal of Mathematical Chemistry*, 51(1): 316–337, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0085-8.

Carbo-Dorca:2013:CED

[2106] Ramon Carbó-Dorca. Collective Euclidian distances and quantum similarity. *Journal of Mathematical Chemistry*, 51(1):338–353, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0086-7.

Zhang:2013:NKS

[2107] Lianzhu Zhang, Shouliu Wei, and Fuliang Lu. The number of Kekulé structures of polyominos on the torus. *Journal of Mathematical Chemistry*, 51(1):354–368, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0087-6.

Nalewajski:2013:UHC

[2108] Roman F. Nalewajski. Use of Harriman's construction in determining molecular equilibrium states. *Journal of Mathematical Chemistry*, 51 (1):369–381, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0088-5; http://link.springer.com/content/pdf/10.1007/s10910-012-0088-5.pdf.

Carbo-Dorca:2013:ESM

[2109] Ramon Carbó-Dorca and Emili Besalú. EMP as a similarity measure: a geometric point of view. *Journal of Mathematical Chemistry*, 51(1):

382–389, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0089-4.

Fang:2013:NOE

[2110] Yonglei Fang, Xiong You, and Qinghe Ming. New optimized explicit modified RKN methods for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 51(1):390–411, January 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0090-y.

Carbo-Dorca:2013:ACC

[2111] Ramon Carbó-Dorca. About the concept of chemical space: a concerned reflection on some trends of modern scientific thought within theoretical chemical lore. *Journal of Mathematical Chemistry*, 51(2):413–419, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0091-x.

Carbo-Dorca:2013:PMH

[2112] Ramon Carbó-Dorca. Position-momentum Heisenberg uncertainty in Gaussian enfoldments of Euclidian space. *Journal of Mathematical Chemistry*, 51(2):420–426, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0094-7.

Paldus:2013:SBI

[2113] Josef Paldus, Tokuei Sako, Xiangzhu Li, and Geerd H. F. Diercksen. Symmetry-breaking in the independent particle model: nature of the singular behavior of Hartree–Fock potentials. *Journal of Mathematical Chemistry*, 51(2):427–450, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0093-8.

Chen:2013:LTB

[2114] Zhenzhen Chen and Tonghua Zhang. Long time behaviour of a stochastic model for continuous flow bioreactor. *Journal of Mathematical Chemistry*, 51(2):451–464, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0095-6.

Milani:2013:EGA

[2115] G. Milani. Effective GA approach for a direct evaluation of reaction kinetic within EPDM accelerated sulphur crosslinking. *Journal of Math-*

ematical Chemistry, 51(2):465–491, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0098-3`.

Skakauskas:2013:NSL

[2116] V. Skakauskas and P. Katauskis. Numerical study of long-range surface diffusion influence on catalytic reactivity of spatially inhomogeneous planar surfaces. *Journal of Mathematical Chemistry*, 51(2):492–502, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0100-0`.

Liu:2013:CBF

[2117] Yue Liu, Ying Liu, and Michael G. B. Drew. Correlation between Fourier series expansion and Hückel orbital theory. *Journal of Mathematical Chemistry*, 51(2):503–531, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0092-9`.

Alolyan:2013:HOF

[2118] Ibraheem Alolyan and T. E. Simos. High order four-step hybrid method with vanished phase-lag and its derivatives for the approximate solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 51(2): 532–555, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0102-y`.

Pereira:2013:ANS

[2119] F. N. Pereira, G. S. L. Andreis, A. L. De Bortoli, and N. R. Marcílio. Analytical-numerical solution for turbulent jet diffusion flames of hydrogen. *Journal of Mathematical Chemistry*, 51(2):556–568, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0101-z`.

Bianchi:2013:BKI

[2120] Monica Bianchi, Alessandra Cornaro, José Luis Palacios, and Anna Torriero. Bounds for the Kirchhoff index via majorization techniques. *Journal of Mathematical Chemistry*, 51(2):569–587, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0103-x`.

Das:2013:EPM

[2121] Biswajit Das, Kinshuk Banerjee, and Gautam Gangopadhyay. Entropy production of a mechanically driven single oligomeric enzyme: a conse-

quence of fluctuation theorem. *Journal of Mathematical Chemistry*, 51 (2):588–602, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0099-2.

Liu:2013:MRP

[2122] Saihua Liu and Jianping Ou. On maximal resonance of polyomino graphs. *Journal of Mathematical Chemistry*, 51(2):603–619, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0104-9.

Romera:2013:REU

[2123] E. Romera, R. del Real, M. Calixto, S. Nagy, and Á. Nagy. Rényi entropy of the u(3) vibron model. *Journal of Mathematical Chemistry*, 51(2): 620–636, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0106-7.

Bie:2013:SPT

[2124] Qunyi Bie and Qiru Wang. Stationary patterns in a two-cell coupled isothermal chemical system with arbitrary powers of autocatalysis. *Journal of Mathematical Chemistry*, 51(2):637–659, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0111-x.

Carbo-Dorca:2013:FES

[2125] Ramon Carbó-Dorca and Emili Besalú. Function extended spaces. *Journal of Mathematical Chemistry*, 51(2):660–671, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0110-y.

Martini:2013:ITD

[2126] Johannes W. R. Martini, Martin Schlather, and G. Matthias Ullmann. On the interaction of two different types of ligands binding to the same molecule part I: basics and the transfer of the decoupled sites representation to systems with n and one binding sites. *Journal of Mathematical Chemistry*, 51(2):672–695, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0107-6; http://link.springer.com/content/pdf/10.1007/s10910-012-0107-6.pdf.

Martini:2013:IDT

[2127] Johannes W. R. Martini, Martin Schlather, and G. Matthias Ullmann. On the interaction of different types of ligands binding to the same molecule. Part II: systems with n to 2 and n to 3 binding sites. *Journal of Mathematical Chemistry*, 51(2):696–714, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0108-5; http://link.springer.com/content/pdf/10.1007/s10910-012-0108-5.pdf`.

Liu:2013:MACa

[2128] Ying Liu, Yue Liu, and Michael G. B. Drew. A mathematical approach to chemical equilibrium theory for gaseous systems — I: theory. *Journal of Mathematical Chemistry*, 51(2):715–740, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0105-8`.

Liu:2013:MACb

[2129] Ying Liu, Yue Liu, and Michael G. B. Drew. A mathematical approach to chemical equilibrium theory for gaseous systems — II: extensions and applications. *Journal of Mathematical Chemistry*, 51(2):741–762, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0109-4`.

Akbari:2013:PFV

[2130] Ali Akbari, Norman H. March, and Angel Rubio. A proposed family of variationally correlated first-order density matrices for spin-polarized three-electron model atoms. *Journal of Mathematical Chemistry*, 51(2):763–773, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0113-8`.

Carbo-Dorca:2013:SCA

[2131] Ramon Carbó-Dorca. Simple comparison of atomic population and shape atomic populations distributions between two molecular structures with a coherent number of atoms. *Journal of Mathematical Chemistry*, 51(2):774–784, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0116-5`.

Li:2013:IRB

[2132] YouNing Li, HuaJun Huang, and Dong Ruan. Indecomposable representations and boson realizations of the nonlinear deformed angular momentum algebra of Witten's first type. *Journal of Mathematical Chemistry*, 51(2):785–809, February 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0114-7`.

Weaver:2013:SEI

[2133] Ian N. Weaver and Donald F. Weaver. A simple electrotopological index for quantitative structure-activity relationship correlation of physical properties with biomolecular activities. *Journal of Mathematical Chemistry*, 51(3):811–816, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0143-x`.

Karimi:2013:RSC

[2134] Sasan Karimi, Marty Lewinter, Michael Kuepfert, and Anthony Delgado. Resonance structure counts in contorted and flat hexabenzocoronenes. *Journal of Mathematical Chemistry*, 51(3):817–825, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0118-3`.

Vogt:2013:AAS

[2135] D. Vogt. On approximate analytical solutions of differential equations in enzyme kinetics using homotopy perturbation method. *Journal of Mathematical Chemistry*, 51(3):826–842, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0121-8`.

Carbo-Dorca:2013:NGP

[2136] Ramon Carbó-Dorca. A naïve geometrical perspective of Fukui functions: definition of Fukui function skew symmetric matrices described on density function sets. *Journal of Mathematical Chemistry*, 51(3):843–856, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0120-9`.

Bielinska-Waz:2013:SPS

[2137] Dorota Bielińska-Waz, Piotr Waz, Timothy Clark, Tomasz Puzyn, Lukasz Peplowski, and Wiesław Nowak. Statistical properties of spectra of chloronaphthalenes. *Journal of Mathematical Chemistry*, 51(3):

857–867, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0117-4; http://link.springer.com/content/pdf/10.1007/s10910-012-0117-4.pdf.

Bucknum:2013:E

[2138] M. J. Bucknum, Dasari L. V. K. Prasad, and E. A. Castro. Exocyclobutadieneite. *Journal of Mathematical Chemistry*, 51(3):868–880, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0115-6.

Jia:2013:NAS

[2139] Ji-Teng Jia and Tomohiro Sogabe. A novel algorithm for solving quasi penta-diagonal linear systems. *Journal of Mathematical Chemistry*, 51(3):881–889, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0122-7.

Merkli:2013:ETR

[2140] M. Merkli, G. P. Berman, and R. Sayre. Electron transfer reactions: generalized spin-boson approach. *Journal of Mathematical Chemistry*, 51(3):890–913, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0124-5.

Miskinis:2013:MLR

[2141] Paulius Miskinis. Modelling linear reactions in inhomogeneous catalytic systems. *Journal of Mathematical Chemistry*, 51(3):914–926, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0125-4.

Zadeh:2013:MAP

[2142] Farnaz Heidar Zadeh and Paul W. Ayers. Molecular alignment as a penalized permutation Procrustes problem. *Journal of Mathematical Chemistry*, 51(3):927–936, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-012-0119-2.

Liu:2013:NME

[2143] Shiwei Liu, Juan Zheng, and Yonglei Fang. A new modified embedded 5(4) pair of explicit Runge–Kutta methods for the numerical solution

of the Schrödinger equation. *Journal of Mathematical Chemistry*, 51 (3):937–953, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0127-2`.

Mukherjee:2013:SETa

[2144] Neetik Mukherjee. A simple and effective technique to variationally interpret the structure of SUSY partners of mirror image potentials. *Journal of Mathematical Chemistry*, 51(3):954–975, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0126-3`.

Oyewumi:2013:BSS

[2145] K. J. Oyewumi, O. J. Oluwadare, K. D. Sen, and O. A. Babalola. Bound state solutions of the Deng–Fan molecular potential with the Pekeris-type approximation using the Nikiforov–Uvarov (N-U) method. *Journal of Mathematical Chemistry*, 51(3):976–991, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0123-6`.

Hariharan:2013:HAM

[2146] G. Hariharan. The homotopy analysis method applied to the Kolmogorov–Petrovskii–Piskunov (KPP) and fractional KPP equations. *Journal of Mathematical Chemistry*, 51(3):992–1000, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0132-5`.

Thamwattana:2013:MIB

[2147] Ngamta Thamwattana, Thien Tran-Duc, and Duangkamon Baowan. Modelling interactions between a PBB and fullerenes. *Journal of Mathematical Chemistry*, 51(3):1001–1022, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0129-0`.

Amore:2013:PCU

[2148] Paolo Amore and Francisco M. Fernández. Particle correlation from uncorrelated non Born–Oppenheimer SCF wavefunctions. *Journal of Mathematical Chemistry*, 51(3):1023–1035, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0133-4`.

Letelier:2013:VSM

[2149] Ricardo D. Letelier. On the variational solution of morphed molecular potential in a diatomic molecule. *Journal of Mathematical Chemistry*, 51 (3):1036–1042, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0135-2`.

Balaban:2013:DHR

[2150] Alexandru T. Balaban. Diamond hydrocarbons revisited: partitioned formula tables of diamondoids. *Journal of Mathematical Chemistry*, 51 (3):1043–1055, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0130-7`.

Merkin:2013:BDR

[2151] J. H. Merkin. A boundary-driven reaction front. *Journal of Mathematical Chemistry*, 51(3):1056–1075, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0137-0`.

Chen:2013:DSM

[2152] Zhenzhen Chen and Tonghua Zhang. Dynamics of a stochastic model for continuous flow bioreactor with Contois growth rate. *Journal of Mathematical Chemistry*, 51(3):1076–1091, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0141-4`.

Carbo-Dorca:2013:ECS

[2153] Ramon Carbó-Dorca. Enfolded conformational spaces: definition of the chemical quantum mechanical multiverse under Born–Oppenheimer approximation. *Journal of Mathematical Chemistry*, 51(3):1092–1098, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0136-1`.

Bofill:2013:AVR

[2154] Josep Maria Bofill and Wolfgang Quapp. Analysis of the valley–ridge inflection points through the partitioning technique of the Hessian eigenvalue equation. *Journal of Mathematical Chemistry*, 51(3): 1099–1115, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0134-3`.

Milani:2013:DMA

[2155] G. Milani and F. Milani. Differential model accounting for reversion for EPDM vulcanized with peroxides. *Journal of Mathematical Chemistry*, 51(3):1116–1133, March 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0140-5`.

Vigo-Aguiar:2013:MMC

[2156] J. Vigo-Aguiar. Mathematical modeling for chemistry-related applications. *Journal of Mathematical Chemistry*, 51(4):1135–1138, April 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0112-9; http://link.springer.com/content/pdf/10.1007/s10910-012-0112-9.pdf`.

Rey-Ronco:2013:TME

[2157] M. A. Rey-Ronco, T. Alonso-Sánchez, J. Coppen-Rodríguez, and M. P. Castro-García. A thermal model and experimental procedure for a point-source approach to determining the thermal properties of drill cuttings. *Journal of Mathematical Chemistry*, 51(4):1139–1152, April 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0097-4`.

Alonso:2013:NLP

[2158] P. Alonso, F. Argüeso, R. Cortina, J. Ranilla, and A. M. Vidal. Nonlinear parallel solver for detecting point sources in CMB maps using Bayesian techniques. *Journal of Mathematical Chemistry*, 51(4):1153–1163, April 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0078-7`.

Lopez:2013:NGR

[2159] Miguel A. López and Raquel Martínez. A note on the generalized Rayleigh equation: limit cycles and stability. *Journal of Mathematical Chemistry*, 51(4):1164–1169, April 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0096-5`.

Demiralp:2013:PEAa

[2160] Metin Demiralp. A probabilistic evolution approach trilogy, part 1: quantum expectation value evolutions, block triangularity and conicality, truncation approximants and their convergence. *Journal of Mathematical Chemistry*, 51(4):1170–1186, April 2013. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0079-6`.

Demiralp:2013:PEAb

[2161] Metin Demiralp and N. A. Baykara. A probabilistic evolution approach trilogy, part 2: spectral issues for block triangular evolution matrix, singularities, space extension. *Journal of Mathematical Chemistry*, 51(4): 1187–1197, April 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0080-0`.

Demiralp:2013:PEAc

[2162] Metin Demiralp and Burcu Tunga. A probabilistic evolution approach trilogy, part 3: temporal variation of state variable expectation values from Liouville equation perspective. *Journal of Mathematical Chemistry*, 51(4):1198–1210, April 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0081-z`.

Kaatz:2013:SPC

[2163] Forrest H. Kaatz and Adhemar Bultheel. Statistical properties of carbon nanostructures. *Journal of Mathematical Chemistry*, 51(5):1211–1220, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0128-1`.

Kaatz:2013:PLS

[2164] Forrest H. Kaatz and Adhemar Bultheel. Power law statistics of rippled graphene nanoflakes. *Journal of Mathematical Chemistry*, 51(5): 1221–1230, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0131-6`.

Dong:2013:ABC

[2165] Qinglai Dong, Wanbiao Ma, and Mingjuan Sun. The asymptotic behavior of a Chemostat model with Crowley–Martin type functional response and time delays. *Journal of Mathematical Chemistry*, 51(5):1231–1248, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0138-z`.

Mackevicius:2013:CMS

[2166] Mazvydas Mackevicius, Feliksas Ivanauskas, Aivaras Kareiva, and Irma Bogdanoviciene. Computer modeling of synthesis of calcium hydroxya-

patite (CHAp). *Journal of Mathematical Chemistry*, 51(5):1249–1257, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-012-0139-y`.

Chan:2013:ISU

[2167] Yue Chan and James M. Hill. Ion selectivity using membranes comprising functionalized carbon nanotubes. *Journal of Mathematical Chemistry*, 51 (5):1258–1273, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0142-y`.

Dong:2013:QAC

[2168] Qinglai Dong and Wanbiao Ma. Qualitative analysis of the chemostat model with variable yield and a time delay. *Journal of Mathematical Chemistry*, 51(5):1274–1292, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0144-9`.

Li:2013:CEA

[2169] Wenliang Li and Keli Han. A comparison of efficiency and accuracy of two-electron integrals calculation between two methods in multi-configuration time-dependent Hartree–Fock frame. *Journal of Mathematical Chemistry*, 51(5):1293–1299, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0145-8`.

DellAcqua:2013:LOA

[2170] Guido Dell'Acqua. Leading order asymptotics in the Goldbeter–Koshland switch. *Journal of Mathematical Chemistry*, 51(5):1300–1309, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0146-7`.

Liu:2013:HPO

[2171] Shuya Liu and Heping Zhang. The HOMFLY polynomials of odd polyhedral links. *Journal of Mathematical Chemistry*, 51(5):1310–1328, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0147-6`.

Deng:2013:EDP

[2172] Kecai Deng, Jianguo Qian, and Fuji Zhang. Enumerating DNA polyhedral links. *Journal of Mathematical Chemistry*, 51(5):1329–1342, May

2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0148-5.

Hwang:2013:BSBa

[2173] Hyung Ju Hwang and Juan J. L. Velázquez. Bistable stochastic biochemical networks: highly specific systems with few chemicals. *Journal of Mathematical Chemistry*, 51(5):1343–1375, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0150-y.

Meremianin:2013:EFH

[2174] A. V. Meremianin. Eckart frame Hamiltonians in the three-body problem. *Journal of Mathematical Chemistry*, 51(5):1376–1387, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0152-9.

Szczepanik:2013:SED

[2175] Dariusz Szczepanik and Janusz Mrozek. Stationarity of electron distribution in ground-state molecular systems. *Journal of Mathematical Chemistry*, 51(5):1388–1396, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0153-8; http://link.springer.com/content/pdf/10.1007/s10910-013-0153-8.pdf.

Carbo-Dorca:2013:VPH

[2176] Ramon Carbó-Dorca. Variational principle, Hohenberg–Kohn theorem, and density function origin shifts. *Journal of Mathematical Chemistry*, 51(5):1397–1409, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0154-7.

Li:2013:NPM

[2177] Risong Li, Xiaoliang Zhou, Yu Zhao, and Cunyou Huang. A note on the principal measure and distributional $(p,\vec{q})$-chaos of a coupled lattice system related with Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 51(5):1410–1417, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0155-6. See comment [2313].

Alolyan:2013:NFSa

[2178] Ibraheem Alolyan and T. E. Simos. A new four-step Runge–Kutta type method with vanished phase-lag and its first, second and third deriva-

tives for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 51(5):1418–1445, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0156-5`.

Nath:2013:ITS

[2179] D. Nath. Information theoretic spreading measures of orthogonal functions. *Journal of Mathematical Chemistry*, 51(5):1446–1461, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0157-4`.

Akbari:2013:EFP

[2180] A. Akbari, C. Amovilli, N. H. March, and A. Rubio. Explicit form of Pauli potential for direct derivation of pair density from a two-particle differential equation for the quintet state of four electrons with harmonic interparticle interactions. *Journal of Mathematical Chemistry*, 51(5): 1462–1466, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0158-3`.

Dhatt:2013:SSE

[2181] Sharmistha Dhatt and Kamal Bhattacharyya. Single-substrate enzyme kinetics: the quasi-steady-state approximation and beyond. *Journal of Mathematical Chemistry*, 51(5):1467–1477, May 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0160-9`.

Jesudason:2013:RCT

[2182] C. G. Jesudason and A. J. P. Agung. Reflections on the conformation, topology and thermodynamics of a polyelectrolyte chain in the presence of counterions with plausible applications. *Journal of Mathematical Chemistry*, 51(6):1479–1514, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0159-2`. See erratum [2235].

Glasser:2013:WHC

[2183] M. L. Glasser, N. H. March, and L. M. Nieto. Weak harmonic confinement of the quintet solution of a Moshinsky atom with 4 electrons. *Journal of Mathematical Chemistry*, 51(6):1515–1520, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0151-x`.

Li:2013:STD

[2184] Wenliang Li. Solving for the time-dependent multi-configuration Hartree–Fock equations based on sine-discrete variable representation. *Journal of Mathematical Chemistry*, 51(6):1521–1531, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0161-8`.

Aydemir:2013:NMM

[2185] Adnan Aydemir, Necmettin Yildirim, Bernd Hitzmann, and Thomas Scheper. A new mathematical model for the enzymatic kinetic resolution of racemates. *Journal of Mathematical Chemistry*, 51(6):1532–1547, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0162-7`.

Grigoriu:2013:CAQ

[2186] A. Grigoriu, H. Rabitz, and G. Turinici. Controllability analysis of quantum systems immersed within an engineered environment. *Journal of Mathematical Chemistry*, 51(6):1548–1560, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0163-6`.

Geldof:2013:CRW

[2187] D. Geldof, C. Van Alsenoy, and N. H. March. The central role of the von Weizsäcker kinetic energy density in determining the energy functional of a model two-electron atom with harmonic confinement and inverse square interparticle repulsion. *Journal of Mathematical Chemistry*, 51 (6):1561–1568, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0164-5`.

Carbo-Dorca:2013:PCD

[2188] Ramon Carbó-Dorca. Particle coordinates and discrete molecular description: a geometric point of view on a twofold dimensionality environment. *Journal of Mathematical Chemistry*, 51(6):1569–1583, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0165-4`.

Andreis:2013:BCB

[2189] G. S. L. Andreis, F. A. Vaz, and A. L. De Bortoli. Bioethanol combustion based on a reduced kinetic mechanism. *Journal of Mathematical*

Chemistry, 51(6):1584–1598, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0166-3`.

Doslic:2013:PPG

[2190] Tomislav Doslić. Planar polycyclic graphs and their Tutte polynomials. *Journal of Mathematical Chemistry*, 51(6):1599–1607, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0167-2`.

Klein:2013:ESH

[2191] D. J. Klein and C. E. Larson. Eigenvalues of saturated hydrocarbons. *Journal of Mathematical Chemistry*, 51(6):1608–1618, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0168-1`.

Szczepanik:2013:QBO

[2192] Dariusz Szczepanik and Janusz Mrozek. On quadratic bond-order decomposition within molecular orbital space. *Journal of Mathematical Chemistry*, 51(6):1619–1633, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0169-0; http://link.springer.com/content/pdf/10.1007/s10910-013-0169-0.pdf`.

Gonzalez-Hernandez:2013:CAN

[2193] J. L. González-Hernández, M. Mar Canedo, and Sonsoles Encinar. Combining artificial neural networks and experimental design to prediction of kinetic rate constants. *Journal of Mathematical Chemistry*, 51(6):1634–1653, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0170-7`.

Skakauskas:2013:PDR

[2194] V. Skakauskas and P. Katauskis. Product desorption rate influence on catalytic reactivity of spatially inhomogeneous surfaces. *Journal of Mathematical Chemistry*, 51(6):1654–1669, June 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0171-6`.

Ugurlu:2013:DOI

[2195] Ekin Ugurlu and Elgiz Bairamov. Dissipative operators with impulsive conditions. *Journal of Mathematical Chemistry*, 51(6):1670–1680, June

2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0172-5.

Carbo-Dorca:2013:DFC

[2196] Ramon Carbó-Dorca. On density function coordinate matrix. *Journal of Mathematical Chemistry*, 51(7):1681–1683, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0186-z.

Toropova:2013:CQE

[2197] A. P. Toropova, A. A. Toropov, E. Benfenati, G. Gini, D. Leszczynska, and J. Leszczynski. CORAL: QSPRs of enthalpies of formation of organometallic compounds. *Journal of Mathematical Chemistry*, 51(7):1684–1693, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0177-0.

March:2013:TPV

[2198] N. H. March and Z. D. Zhang. Theory and phenomenology for a variety of classical and quantum phase transitions. *Journal of Mathematical Chemistry*, 51(7):1694–1711, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0181-4.

Li:2013:PMD

[2199] Risong Li, Fu Huang, Yu Zhao, Zengxiong Chen, and Cunyou Huang. The principal measure and distributional (p, q)-chaos of a coupled lattice system with coupling constant $\varepsilon = 1$ related with Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 51(7):1712–1719, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0174-3.

Shu:2013:IDM

[2200] Jian-Jun Shu and Kian Yan Yong. Identifying DNA motifs based on match and mismatch alignment information. *Journal of Mathematical Chemistry*, 51(7):1720–1728, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0175-2.

Patricio:2013:RSF

[2201] M. Patrício, J. L. Santos, F. Patrício, and A. J. C. Varandas. Roadmap to spline-fitting potentials in high dimensions. *Journal of Mathematical*

Chemistry, 51(7):1729–1746, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0173-4`.

Cai:2013:QHM

[2202] Zhenning Cai, Yuwei Fan, Ruo Li, Tiao Lu, and Wenqi Yao. Quantum hydrodynamic model of density functional theory. *Journal of Mathematical Chemistry*, 51(7):1747–1771, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0176-1`.

Besalu:2013:CSM

[2203] Emili Besalú and Ramon Carbó-Dorca. Completely soft molecular electrostatic potentials (CoSMEP) and total density functions. *Journal of Mathematical Chemistry*, 51(7):1772–1783, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0180-5`.

Tuna:2013:NPM

[2204] Süha Tuna and Burcu Tunga. A novel piecewise multivariate function approximation method via universal matrix representation. *Journal of Mathematical Chemistry*, 51(7):1784–1801, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0179-y`.

Neto:2013:MNG

[2205] Antônio Francisco Neto. Matula numbers, Gödel numbering and Fock space. *Journal of Mathematical Chemistry*, 51(7):1802–1814, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0178-z`.

Reuben:2013:PSM

[2206] A. Merwyn Jasper D. Reuben, Dinesh Varshney, and K. Jayakumar. The possibility of semiconductor-metal transition in a spherical quantum dot. *Journal of Mathematical Chemistry*, 51(7):1815–1821, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0183-2`.

Miskinis:2013:ETS

[2207] P. Miskinis. An example of a two-stage chemical reaction whose kinetics may be found in an analytical form. *Journal of Mathematical Chemistry*, 51(7):1822–1834, August 2013. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0185-0`.

Morales-Bayuelo:2013:TMP

[2208] Alejandro Morales-Bayuelo and Ricardo Vivas-Reyes. Theoretical model for the polarization molecular and Hückel treatment of phosphocyclopentadiene in an external electric field: Hirschfeld study. *Journal of Mathematical Chemistry*, 51(7):1835–1852, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0182-3`.

Flapan:2013:ICM

[2209] Erica Flapan and Will Fletcher. Intrinsic chirality of multipartite graphs. *Journal of Mathematical Chemistry*, 51(7):1853–1863, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0187-y`.

Carrero-Mantilla:2013:ESS

[2210] J. Carrero-Mantilla and S. Duque-Tobón. Efficient stochastic simulation of simultaneous reaction and diffusion in a gas-liquid interface. *Journal of Mathematical Chemistry*, 51(7):1864–1880, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0188-x`.

Sesma:2013:ESS

[2211] J. Sesma. Exact solution of the Schrödinger equation with a Lennard-Jones potential. *Journal of Mathematical Chemistry*, 51(7):1881–1896, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0189-9`.

Thilagam:2013:CBF

[2212] A. Thilagam. Crossover from bosonic to fermionic features in composite boson systems. *Journal of Mathematical Chemistry*, 51(7):1897–1913, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0190-3`.

Panopoulos:2013:NOS

[2213] G. A. Panopoulos and T. E. Simos. A new optimized symmetric 8-step semi-embedded predictor-corrector method for the numerical solution of the radial Schrödinger equation and related orbital problems. *Journal of*

Mathematical Chemistry, 51(7):1914–1937, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0184-1`.

Mukherjee:2013:SETb

[2214] Neetik Mukherjee. A simple and effective technique to locate quasi-degeneracy in a symmetric double well potential. *Journal of Mathematical Chemistry*, 51(7):1938–1944, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0192-1`.

Lee:2013:MHP

[2215] Chang Hyeong Lee, Kyung Duk Park, and Bongsoo Jang. Multistage homotopy perturbation method for nonlinear reaction networks. *Journal of Mathematical Chemistry*, 51(7):1945–1960, August 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0195-y`.

Gomez-Reyes:2013:AFD

[2216] José Félix Gómez-Reyes and Armando Ariza-Castolo. Aliasing functions and a dynamic approach to optimizing spectral widths in 2D experiments. *Journal of Mathematical Chemistry*, 51(8):1961–1980, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0191-2`.

Graver:2013:CFN

[2217] Jack E. Graver, Elizabeth J. Hartung, and Ahmed Y. Souid. Clar and Fries numbers for benzenoids. *Journal of Mathematical Chemistry*, 51(8):1981–1989, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0193-0`.

Romero:2013:NHH

[2218] Juan M. Romero, O. González-Gaxiola, and R. Bernal-Jaquez. Non-Hermitian hydrogen atom. *Journal of Mathematical Chemistry*, 51(8):1990–2000, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0194-z`.

Liu:2013:BAR

[2219] Ping Liu, Junping Shi, Yuwen Wang, and Xiuhong Feng. Bifurcation analysis of reaction-diffusion Schnakenberg model. *Journal of Math-*

ematical Chemistry, 51(8):2001–2019, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0196-x`.

AlGaralleh:2013:MIB

[2220] Hakim Al Garalleh, Ngamta Thamwattana, Barry J. Cox, and James M. Hill. Modelling interaction between ammonia and nitric oxide molecules and aquaporins. *Journal of Mathematical Chemistry*, 51(8):2020–2032, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0197-9`.

Milani:2013:CFA

[2221] G. Milani. Closed form analytical approach for a second order nonlinear ODE interpreting EPDM vulcanization with peroxides. *Journal of Mathematical Chemistry*, 51(8):2033–2061, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0198-8`.

Marmorino:2013:CUT

[2222] M. G. Marmorino. Comparison and union of the Temple and Bazley lower bounds. *Journal of Mathematical Chemistry*, 51(8):2062–2073, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0199-7`.

Hwang:2013:BSBb

[2223] Hyung Ju Hwang and Juan J. L. Velázquez. Bistable stochastic biochemical networks: large chemical networks and systems with many molecules. *Journal of Mathematical Chemistry*, 51(8):2074–2103, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0200-5`.

Strekalov:2013:RVN

[2224] M. L. Strekalov. Relaxation of vibrational nonequilibrium distributions: the effect of multiphoton excitation on relaxation behavior. *Journal of Mathematical Chemistry*, 51(8):2104–2119, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0201-4`.

DeBlasio:2013:MDS

[2225] Cataldo De Blasio, Claudio Carletti, Tapio Westerlund, and Mika Järvinen. On modeling the dissolution of sedimentary rocks in acidic

environments. An overview of selected mathematical methods with presentation of a case study. *Journal of Mathematical Chemistry*, 51(8): 2120–2143, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0202-3`.

Anbumalar:2013:AOC

[2226] S. Anbumalar, R. Ananda Natarajan, and P. Rameshbabu. An algorithm for overlapped chromatogram separation. *Journal of Mathematical Chemistry*, 51(8):2144–2164, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0203-2`.

Jia:2013:EDR

[2227] Chun-Sheng Jia, Tao Chen, Liang-Zhong Yi, and Shu-Rong Lin. Equivalence of the deformed Rosen–Morse potential energy model and Tietz potential energy model. *Journal of Mathematical Chemistry*, 51(8): 2165–2172, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0204-1`.

Li:2013:NLY

[2228] Risong Li, Fu Huang, and Yu Zhao. A note on Li–Yorke chaos in a coupled lattice system related with Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 51(8):2173–2178, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0205-0`.

Petrov:2013:FIP

[2229] D. N. Petrov and B. M. Angelov. Free ions Pr IV ($4f^2$) and Tm IV ($4f^{12}$): intermediate versus LS coupling scheme. *Journal of Mathematical Chemistry*, 51(8):2179–2186, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0206-z`.

Tasi:2013:VAM

[2230] Gyula Tasi, László Nagy-Gyevi, Roland Tóbiás, and Tamás S. Tasi. Vector algebra and molecular symmetry: a tribute to Professor Josiah Willard Gibbs. *Journal of Mathematical Chemistry*, 51(8):2187–2195, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0207-y`.

Arpat:2013:EEN

[2231] Esra Kir Arpat. An eigenfunction expansion of the non-selfadjoint Sturm–Liouville operator with a singular potential. *Journal of Mathematical Chemistry*, 51(8):2196–2213, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0208-x`.

Ray:2013:SST

[2232] S. Saha Ray. Soliton solutions for time fractional coupled modified KdV equations using new coupled fractional reduced differential transform method. *Journal of Mathematical Chemistry*, 51(8):2214–2229, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0210-3`.

Toropova:2013:ODT

[2233] Alla P. Toropova, Andrey A. Toropov, Tomasz Puzyn, Emilio Benfenati, Danuta Leszczynska, and Jerzy Leszczynski. Optimal descriptor as a translator of eclectic information into the prediction of thermal conductivity of micro-electro-mechanical systems. *Journal of Mathematical Chemistry*, 51(8):2230–2237, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0211-2`.

Perovic:2013:NAP

[2234] Vladimir R. Perović. Novel algorithm for phylogenetic analysis of proteins: application to analysis of the evolution of H5N1 influenza viruses. *Journal of Mathematical Chemistry*, 51(8):2238–2255, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0212-1`.

Jesudason:2013:ERC

[2235] C. G. Jesudason and A. A. J. Agung. Erratum to: Reflections on the conformation, topology and thermodynamics of a polyelectrolyte chain in the presence of counterions with plausible applications. *Journal of Mathematical Chemistry*, 51(8):2256, September 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0209-9; http://link.springer.com/content/pdf/10.1007/s10910-013-0209-9.pdf`. See [2182].

Vogt:2013:SPS

[2236] D. Vogt. A simplified perturbation solution of Michaelis–Menten kinetics equations in a "total" framework. *Journal of Mathematical Chemistry*, 51(9):2257–2263, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0221-0`.

Benassi:2013:ARP

[2237] Enrico Benassi. Application of Redfield–Pólya's theorem to the enumeration of the substitution isomers of linear polycyclic aromatic hydrocarbons. *Journal of Mathematical Chemistry*, 51(9):2264–2270, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0242-8`.

Michel:2013:SCW

[2238] Denis Michel and Philippe Ruelle. Seven competing ways to recover the Michaelis–Menten equation reveal the alternative approaches to steady state modeling. *Journal of Mathematical Chemistry*, 51(9):2271–2284, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0237-5`.

Wal:2013:EBF

[2239] Andrzej Wal. Energy bands for finite two-dimensional systems in a quantised magnetic field: the symmetry of the model. *Journal of Mathematical Chemistry*, 51(9):2285–2316, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0225-9`.

AlGaralleh:2013:MCD

[2240] Hakim Al Garalleh, Ngamta Thamwattana, Barry J. Cox, and James M. Hill. Modelling carbon dioxide molecule interacting with aquaglyceroporin and aquaporin-1 channels. *Journal of Mathematical Chemistry*, 51(9):2317–2327, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0240-x`.

Thongchuay:2013:MAM

[2241] Watcharakorn Thongchuay, Puntip Toghaw, and Montri Maleewong. Multilevel augmentation method with wavelet bases for singularly perturbed problem. *Journal of Mathematical Chemistry*, 51(9):2328–2339, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0213-0.

Huang:2013:RAB

[2242] ZaiTang Huang and ChunTao Chen. Random attractions and bifurcation for the classical Rayleigh–van der Pol equations with small noise. *Journal of Mathematical Chemistry*, 51(9):2340–2353, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0214-z; http://link.springer.com/content/pdf/10.1007/s10910-013-0214-z.pdf.

Fulop:2013:TDC

[2243] Ottilia Fülöp and Béla Barabás. Three-dimensional chiral objects and their star graph representations. *Journal of Mathematical Chemistry*, 51(9):2354–2360, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0215-y.

Mahalakshmi:2013:WML

[2244] M. Mahalakshmi, G. Hariharan, and K. Kannan. The wavelet methods to linear and nonlinear reaction-diffusion model arising in mathematical chemistry. *Journal of Mathematical Chemistry*, 51(9):2361–2385, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0216-x.

Hariharan:2013:NCW

[2245] G. Hariharan and R. Rajaraman. A new coupled wavelet-based method applied to the nonlinear reaction-diffusion equation arising in mathematical chemistry. *Journal of Mathematical Chemistry*, 51(9):2386–2400, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0217-9.

Rao:2013:GTA

[2246] Shodhan Rao, Arjan van der Schaft, and Bayu Jayawardhana. A graph-theoretical approach for the analysis and model reduction of complex-balanced chemical reaction networks. *Journal of Mathematical Chemistry*, 51(9):2401–2422, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0218-8.

Kuperkar:2013:SIO

[2247] Rakhee Kuperkar and D. M. Patel. Surfactant induced one dimensional unsaturated flow through porous media: a classical mathematical approach. *Journal of Mathematical Chemistry*, 51(9):2423–2431, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0219-7`.

Hariharan:2013:TRW

[2248] G. Hariharan and R. Rajaraman. Two reliable wavelet methods to Fitzhugh–Nagumo (FN) and fractional FN equations. *Journal of Mathematical Chemistry*, 51(9):2432–2454, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0220-1`.

Boros:2013:DEP

[2249] Balázs Boros. On the dependence of the existence of the positive steady states on the rate coefficients for deficiency-one mass action systems: single linkage class. *Journal of Mathematical Chemistry*, 51(9):2455–2490, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0222-z`.

Meskauskas:2013:DSA

[2250] Tadas Meskauskas, Feliksas Ivanauskas, and Valdas Laurinavicius. Degradation of substrate and/or product: mathematical modeling of biosensor action. *Journal of Mathematical Chemistry*, 51(9):2491–2502, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0223-y`.

Jiang:2013:DEQ

[2251] Yao-Lin Jiang and Ji-Teng Jia. On the determinant evaluation of quasi penta-diagonal matrices and quasi penta-diagonal Toeplitz matrices. *Journal of Mathematical Chemistry*, 51(9):2503–2513, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0224-x`.

Nesterov:2013:NAQ

[2252] Alexander I. Nesterov, Gennady P. Berman, José Manuel Sánchez Martínez, and Richard T. Sayre. Noise-assisted quantum electron

transfer in photosynthetic complexes. *Journal of Mathematical Chemistry*, 51(9):2514–2541, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0226-8`.

Alolyan:2013:NFSb

[2253] Ibraheem Alolyan and T. E. Simos. A new four-step hybrid type method with vanished phase-lag and its first derivatives for each level for the approximate integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 51(9):2542–2571, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0227-7`.

Belkic:2013:MDS

[2254] Dzevad Belkić and Karen Belkić. Mechanistic description of survival of irradiated cells: repair kinetics in Padé linear-quadratic or differential Michaelis–Menten model. *Journal of Mathematical Chemistry*, 51(9):2572–2607, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0243-7`.

Belkic:2013:REK

[2255] Dzevad Belkić and Karen Belkić. Resolution enhancement as a key step towards clinical implementation of Padé-optimized magnetic resonance spectroscopy for diagnostic oncology. *Journal of Mathematical Chemistry*, 51(9):2608–2637, October 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0244-6`.

Rosenfeld:2013:AFT

[2256] Vladimir R. Rosenfeld. Another form of the transmission function. *Journal of Mathematical Chemistry*, 51(10):2639–2643, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0239-3`.

Rosenfeld:2013:SSC

[2257] Vladimir R. Rosenfeld. Selfcomplementary, selfreverse cyclic nucleotide sequences codonically invariant under frame shifting. *Journal of Mathematical Chemistry*, 51(10):2644–2653, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0238-4`.

Tunga:2013:NMM

[2258] M. Alper Tunga and Metin Demiralp. A novel method for multivariate data modelling: Piecewise generalized EMPR. *Journal of Mathematical Chemistry*, 51(10):2654–2667, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0228-6`.

Li:2013:QSS

[2259] Bo Li and Banghe Li. Quasi-steady-state laws in reversible model of enzyme kinetics. *Journal of Mathematical Chemistry*, 51(10):2668–2686, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0229-5`.

Szczepanik:2013:MSM

[2260] Dariusz Szczepanik and Janusz Mrozek. Minimal set of molecule-adapted atomic orbitals from maximum overlap criterion. *Journal of Mathematical Chemistry*, 51(10):2687–2698, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0230-z; http://link.springer.com/content/pdf/10.1007/s10910-013-0230-z.pdf`.

Mamedov:2013:AEM

[2261] B. A. Mamedov. Analytical evaluation of the Marcus–Hush–Chidsey function using binomial expansion theorem and error functions. *Journal of Mathematical Chemistry*, 51(10):2699–2703, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0231-y`.

Roy:2013:MCI

[2262] Priti Kumar Roy, Sumit Nandi, and Mithun Kumar Ghosh. Modeling of a control induced system for product formation in enzyme kinetics. *Journal of Mathematical Chemistry*, 51(10):2704–2717, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0232-x`.

Raychaudhury:2013:ICM

[2263] Chandan Raychaudhury and Debnath Pal. Information content of molecular graph and prediction of gas phase thermal entropy of organic compounds. *Journal of Mathematical Chemistry*, 51(10):2718–2730, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (elec-

tronic). URL http://link.springer.com/article/10.1007/s10910-013-0233-9.

Banerjee:2013:RVE

[2264] Kinshuk Banerjee and Gautam Gangopadhyay. Realization of vibronic entanglement in terms of tunneling current in an artificial molecule. *Journal of Mathematical Chemistry*, 51(10):2731–2745, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0234-8.

Tikhonov:2013:QAP

[2265] Nikolay A. Tikhonov and Gleb B. Sidelnikov. Quantitative analysis of physical factors that determine the behavior of activity coefficients of electrolytes. *Journal of Mathematical Chemistry*, 51(10):2746–2756, November 2013. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0235-7.

Cioslowski:2014:NAI

[2266] Jerzy Cioslowski. Note on the asymptotic isomer count of large fullerenes. *Journal of Mathematical Chemistry*, 52(1):1–5, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0263-3; http://link.springer.com/content/pdf/10.1007/s10910-013-0263-3.pdf.

Staskiewicz:2014:AMM

[2267] Beata Staśkiewicz and Wojciech Okrasiński. On approximate mathematical modeling of the vapor–liquid coexistence curves by the van der Waals equation of state and non-classical value of the critical exponent. *Journal of Mathematical Chemistry*, 52(1):6–22, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0236-6.

Cheng:2014:HPD

[2268] Xiao-Sheng Cheng, Yujuan Lei, and Weiling Yang. The Homfly polynomial of double crossover links. *Journal of Mathematical Chemistry*, 52 (1):23–41, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0241-9.

Nalewajski:2014:CML

[2269] Roman F. Nalewajski. Communications in molecules: local and multiconfiguration channels and their entropic descriptors of bond multiplicity

and composition. *Journal of Mathematical Chemistry*, 52(1):42–71, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0245-5; http://link.springer.com/content/pdf/10.1007/s10910-013-0245-5.pdf.

Nalewajski:2014:PIL

[2270] Roman F. Nalewajski. On phases and interference of local communications in molecules. *Journal of Mathematical Chemistry*, 52(1):72–92, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0246-4; http://link.springer.com/content/pdf/10.1007/s10910-013-0246-4.pdf.

Nagy:2014:QFI

[2271] Ilona Nagy and János Tóth. Quadratic first integrals of kinetic differential equations. *Journal of Mathematical Chemistry*, 52(1):93–114, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0247-3.

Dulf:2014:MIS

[2272] Eva-Henrietta Dulf, Cristina I. Muresan, and Mihaela L. Unguresan. Modeling the (^{15}n) isotope separation column. *Journal of Mathematical Chemistry*, 52(1):115–131, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0248-2.

Waz:2014:DDG

[2273] Piotr Waz, Dorota Bielińska-Waz, and Ashesh Nandy. Descriptors of 2D-dynamic graphs as a classification tool of DNA sequences. *Journal of Mathematical Chemistry*, 52(1):132–140, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0249-1; http://link.springer.com/content/pdf/10.1007/s10910-013-0249-1.pdf.

Quevedo:2014:GDC

[2274] Hernando Quevedo and Diego Tapias. Geometric description of chemical reactions. *Journal of Mathematical Chemistry*, 52(1):141–161, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0250-8.

Mikulski:2014:CLO

[2275] Damian Mikulski, Marcin Molski, Jerzy Konarski, and Krzysztof Eder. The construction of ladder operators and coherent states for the Wei hua anharmonic oscillator using the supersymmetric quantum mechanics. *Journal of Mathematical Chemistry*, 52(1):162–173, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0251-7; http://link.springer.com/content/pdf/10.1007/s10910-013-0251-7.pdf`.

Fernandez:2014:PTC

[2276] Francisco M. Fernández. Perturbation theory for confined systems. *Journal of Mathematical Chemistry*, 52(1):174–177, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0252-6`.

Zahed:2014:NAM

[2277] Reza Zahed and Hesam Sharifi. A new approach to maturity of molecules by rationality of finite groups. *Journal of Mathematical Chemistry*, 52 (1):178–187, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0253-5`.

Agarwalla:2014:DDI

[2278] Bijay K. Agarwalla, Sainyam Galhotra, and J. K. Bhattacharjee. Diffusion driven instability to a drift driven one: Turing patterns in the presence of an electric field. *Journal of Mathematical Chemistry*, 52 (1):188–197, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0254-4`.

Randic:2014:CLP

[2279] Milan Randić and Rok Orel. Canonical labels for protein spots of proteomics maps. *Journal of Mathematical Chemistry*, 52(1):198–212, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0255-3`.

Stanic:2014:TDA

[2280] Marija P. Stanić and Ivan Gutman. Towards a definition of almost-equienergetic graphs. *Journal of Mathematical Chemistry*, 52(1):213–221, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0256-2.

Mallory:2014:TTD

[2281] Kristina Mallory and Robert A. Van Gorder. A transformed time-dependent Michaelis–Menten enzymatic reaction model and its asymptotic stability. *Journal of Mathematical Chemistry*, 52(1):222–230, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0257-1.

Dhatt:2014:AEA

[2282] Sharmistha Dhatt and Kamal Bhattacharyya. Accurate estimates of asymptotic indices via fractional calculus. *Journal of Mathematical Chemistry*, 52(1):231–239, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0258-0.

Fang:2014:NOT

[2283] Yonglei Fang and Xiong You. New optimized two-derivative Runge–Kutta type methods for solving the radial Schrödinger equation. *Journal of Mathematical Chemistry*, 52(1):240–254, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0259-z.

Rach:2014:SCL

[2284] Randolph Rach, Jun-Sheng Duan, and Abdul-Majid Wazwaz. Solving coupled Lane–Emden boundary value problems in catalytic diffusion reactions by the Adomian decomposition method. *Journal of Mathematical Chemistry*, 52(1):255–267, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0260-6.

Morneau:2014:ACM

[2285] Brandy N. Morneau, Jaclyn M. Kubala, Carl Barratt, and Pauline M. Schwartz. Analysis of a chemical model system leading to chiral symmetry breaking: Implications for the evolution of homochirality. *Journal of Mathematical Chemistry*, 52(1):268–282, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0261-5.

Dehesa:2014:ANH

[2286] J. S. Dehesa, A. Guerrero, J. L. López, and P. Sánchez-Moreno. Asymptotics ($p \to \infty$) of L_p-norms of hypergeometric orthogonal polynomials.

Journal of Mathematical Chemistry, 52(1):283–300, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0262-4`.

Avery:2014:MIS

[2287] James Emil Avery and John Scales Avery. Molecular integrals for Slater type orbitals using Coulomb Sturmians. *Journal of Mathematical Chemistry*, 52(1):301–312, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0264-2`.

Zhao:2014:SFS

[2288] Xuezhuang Zhao, Jianxia Cui, Zucheng Li, Zhenfeng Shang, Xiufang Xu, Shengkai Xing, Guichang Wang, and Ruifang Li. Symmetries and fuzzy symmetries of carbon nanotubes. *Journal of Mathematical Chemistry*, 52 (1):313–354, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0266-0`.

Padmanabhan:2014:GSA

[2289] A. S. Padmanabhan. Growing self avoiding walk trees. *Journal of Mathematical Chemistry*, 52(1):355–367, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0267-z`.

Biring:2014:NAM

[2290] Shyamal Kumar Biring, Rahul Sharma, and Pinaki Chaudhury. A new adaptive mutation simulated annealing algorithm: application to the study of pure and mixed Pt–Pd clusters. *Journal of Mathematical Chemistry*, 52(1):368–397, January 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0268-y`.

Chikayama:2014:SMC

[2291] Eisuke Chikayama, Yasuhiro Sunaga, Shigeho Noda, and Hideo Yokota. Solvable model for chemical oscillations. *Journal of Mathematical Chemistry*, 52(2):399–406, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0275-z`.

Donovan:2014:LTL

[2292] Ashley Donovan, Vincent Beltrani, and Herschel Rabitz. Local topology at limited resource induced suboptimal traps on the quantum control

landscape. *Journal of Mathematical Chemistry*, 52(2):407–429, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0269-x`.

McNealy:2014:EPN

[2293] Benjamin E. McNealy and Joshua L. Hertz. Extended Poisson–Nernst–Planck modeling of membrane blockage via insoluble reaction products. *Journal of Mathematical Chemistry*, 52(2):430–440, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0270-4`.

CostaReis:2014:CTA

[2294] Martina Costa Reis, Yongqi Wang, and Adalberto Bono Maurizio Sacchi Bassi. A continuum thermodynamical approach to electrochemical systems. *Journal of Mathematical Chemistry*, 52(2):441–463, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0271-3`.

Milani:2014:ECF

[2295] G. Milani and F. Milani. Effective closed form starting point determination for kinetic model interpreting NR vulcanized with sulphur. *Journal of Mathematical Chemistry*, 52(2):464–488, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0272-2`.

Tiangtrong:2014:EBN

[2296] Prangsai Tiangtrong and Duangkamon Baowan. Encapsulation behaviours of nanoparticles entering two-section carbon nanotubes. *Journal of Mathematical Chemistry*, 52(2):489–503, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0273-1`.

Johannessen:2014:ESO

[2297] Kim Johannessen. The exact solution to the one-dimensional Poisson–Boltzmann equation with asymmetric boundary conditions. *Journal of Mathematical Chemistry*, 52(2):504–507, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0274-0`.

Fujita:2014:SIEa

[2298] Shinsaku Fujita. Symmetry-itemized enumeration of quadruplets of RS-stereoisomers: I — The fixed-point matrix method of the USCI approach

combined with the stereoisogram approach. *Journal of Mathematical Chemistry*, 52(2):508–542, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0276-y`.

Fujita:2014:SIEb

[2299] Shinsaku Fujita. Symmetry-itemized enumeration of quadruplets of RS-stereoisomers. II. The partial-cycle-index method of the USCI approach combined with the stereoisogram approach. *Journal of Mathematical Chemistry*, 52(2):543–574, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0277-x`.

Wallner:2014:ALN

[2300] Jakob Wallner, Manfred Kühleitner, Norbert Brunner, Gabriele Lhota, and Karola Vorauer-Uhl. Application of the log-normal model for long term high affinity antibody/antigen interactions using bio-layer interferometry. *Journal of Mathematical Chemistry*, 52(2):575–587, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0278-9`.

Nalewajski:2014:PEM

[2301] Roman F. Nalewajski. On phase-equilibria in molecules. *Journal of Mathematical Chemistry*, 52(2):588–612, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0280-2; http://link.springer.com/content/pdf/10.1007/s10910-013-0280-2.pdf`.

Wazwaz:2014:VIM

[2302] Abdul-Majid Wazwaz. The variational iteration method for solving the Volterra integro-differential forms of the Lane–Emden equations of the first and the second kind. *Journal of Mathematical Chemistry*, 52(2):613–626, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0281-1`.

Padmanabhan:2014:SAW

[2303] A. S. Padmanabhan and Susamma Jacob. Self avoiding walk trees and laces. *Journal of Mathematical Chemistry*, 52(2):627–645, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0283-z`.

Coelho:2014:BSP

[2304] Daniela V. Coelho and João Brandão. Building symmetric polynomials to fit a potential energy surface: application to an A_2B_2 molecule. *Journal of Mathematical Chemistry*, 52(2):646–653, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0284-y`.

Quapp:2014:LSP

[2305] Wolfgang Quapp and Josep Maria Bofill. Level sets as progressing waves: an example for wake-free waves in every dimension. *Journal of Mathematical Chemistry*, 52(2):654–664, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0286-9`.

Martini:2014:DGC

[2306] Johannes W. R. Martini, Michael Habeck, and Martin Schlather. A derivation of the grand canonical partition function for systems with a finite number of binding sites using a Markov chain model for the dynamics of single molecules. *Journal of Mathematical Chemistry*, 52(2): 665–674, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0287-8; http://link.springer.com/content/pdf/10.1007/s10910-013-0287-8.pdf`.

Crofts:2014:SMD

[2307] Jonathan J. Crofts and Ernesto Estrada. A statistical mechanics description of environmental variability in metabolic networks. *Journal of Mathematical Chemistry*, 52(2):675–688, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0288-7`.

Ivanauskas:2014:MMB

[2308] Feliksas Ivanauskas, Pranas Katauskis, and Valdas Laurinavicius. Mathematical modeling of biosensor action in the region between diffusion and kinetic modes. *Journal of Mathematical Chemistry*, 52(2):689–702, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0289-6`.

Balasubramanian:2014:GHP

[2309] Krishnan Balasubramanian. Generalization of the Harary–Palmer power group theorem to all irreducible representations of object and color

groups — color combinatorial group theory. *Journal of Mathematical Chemistry*, 52(2):703–728, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0290-0`.

Horvat:2014:RHP

[2310] Boris Horvat, Gasper Jaklic, Iztok Kavkler, and Milan Randić. Rank of Hadamard powers of Euclidean distance matrices. *Journal of Mathematical Chemistry*, 52(2):729–740, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0291-z`.

Banerjee:2014:MCB

[2311] Kinshuk Banerjee. A model of cooperativity based on restricted binding: kinetic and thermodynamic analysis. *Journal of Mathematical Chemistry*, 52(2):741–753, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0292-y`.

Huang:2014:DSL

[2312] Zaitang Huang, Junfei Cao, and Ting Jiang. Dynamics of stochastic Lorenz family of chaotic systems with jump. *Journal of Mathematical Chemistry*, 52(2):754–774, February 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0293-x; http://link.springer.com/content/pdf/10.1007/s10910-013-0293-x.pdf`.

Li:2014:CNP

[2313] Risong Li. Comment on "A note on the principal measure and distributional (p, q)-chaos of a coupled lattice system related with Belusov–Zhabotinskii reaction". *Journal of Mathematical Chemistry*, 52(3):775–780, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0310-8`. See [2177].

Bujotzek:2014:ZEC

[2314] Alexander Bujotzek, Ole Schütt, Adam Nielsen, Konstantin Fackeldey, and Marcus Weber. ZIBgridfree: efficient conformational analysis by partition-of-unity coupling. *Journal of Mathematical Chemistry*, 52(3):781–804, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0265-1`.

Schutte:2014:LSA

[2315] Michael Schutte and Matthias Dehmer. Large-scale analysis of structural branching measures. *Journal of Mathematical Chemistry*, 52(3): 805–819, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0294-9`.

Banerjee:2014:EPU

[2316] Kinshuk Banerjee and Kamal Bhattacharyya. Entropy production as a universal functional of reaction rate: chemical networks close to steady states. *Journal of Mathematical Chemistry*, 52(3):820–832, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0295-8`.

Simos:2014:EFS

[2317] T. E. Simos. An explicit four-step method with vanished phase-lag and its first and second derivatives. *Journal of Mathematical Chemistry*, 52 (3):833–855, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0296-7`.

Metsidik:2014:SCP

[2318] Metrose Metsidik. Semi-Cartesian product of graphs. *Journal of Mathematical Chemistry*, 52(3):856–865, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0297-6`.

Gozukirmizi:2014:PEAa

[2319] Cosar Gözükirmizi and Metin Demiralp. Probabilistic evolution approach for the solution of explicit autonomous ordinary differential equations. Part 1: Arbitrariness and equipartition theorem in Kronecker power series. *Journal of Mathematical Chemistry*, 52(3):866–880, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0298-5`.

Gozukirmizi:2014:PEAb

[2320] Cosar Gözükirmizi and Metin Demiralp. Probabilistic evolution approach for the solution of explicit autonomous ordinary differential equations. Part 2: Kernel separability, space extension, and, series solution via telescopic matrices. *Journal of Mathematical Chemistry*, 52 (3):881–898, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0299-4`.

Demirplak:2014:UEH

[2321] Mustafa Demirplak. Uniqueness of equilibrium in the Haber synthesis of ammonia. *Journal of Mathematical Chemistry*, 52(3):899–916, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0300-2`.

Alolyan:2014:RKT

[2322] Ibraheem Alolyan and T. E. Simos. A Runge–Kutta type four-step method with vanished phase-lag and its first and second derivatives for each level for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 52(3):917–947, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0301-1`.

Tarko:2014:EDM

[2323] Laszlo Tarko. The effect of the diversity of molecules in sets and similarity of sets on the quality of prediction in QSAR studies. *Journal of Mathematical Chemistry*, 52(3):948–965, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0302-0`.

Koga:2014:EPS

[2324] Toshikatsu Koga. Electron-pair shell density approximation applied to inner and outer densities of atoms. *Journal of Mathematical Chemistry*, 52(3):966–976, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0303-z`.

Graver:2014:KB

[2325] Jack E. Graver and Elizabeth J. Hartung. Kekuléan benzenoids. *Journal of Mathematical Chemistry*, 52(3):977–989, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0304-y`.

Hartung:2014:CCC

[2326] Elizabeth J. Hartung. Clar chains and a counterexample. *Journal of Mathematical Chemistry*, 52(3):990–1006, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0305-5`.

Oldham:2014:PRT

[2327] Keith B. Oldham. The propagation of radiation through a medium containing a component that absorbs the radiation and is steadily destroyed by it. *Journal of Mathematical Chemistry*, 52(3):1007–1019, March 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0309-1`.

Vigo-Aguiar:2014:ADE

[2328] J. Vigo-Aguiar. Applied differential equations and related computational mathematics in chemistry. *Journal of Mathematical Chemistry*, 52(4): 1021–1022, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0340-2; http://link.springer.com/content/pdf/10.1007/s10910-014-0340-2.pdf`.

Canto:2014:ICS

[2329] B. Cantó, C. Coll, E. Sánchez, S. C. Cardona, and J. Navarro-Laboulais. On identifiability for chemical systems from measurable variables. *Journal of Mathematical Chemistry*, 52(4):1023–1035, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0149-4`.

Bayon:2014:OCL

[2330] L. Bayón, J. M. Grau, M. M. Ruiz, and P. M. Suárez. Optimal control of a linear unbranched chemical process with n steps: the quasi-analytical solution. *Journal of Mathematical Chemistry*, 52(4):1036–1049, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0279-8`.

Vigo-Aguiar:2014:SSF

[2331] J. Vigo-Aguiar and Higinio Ramos. A strategy for selecting the frequency in trigonometrically-fitted methods based on the minimization of the local truncation errors and the total energy error. *Journal of Mathematical Chemistry*, 52(4):1050–1058, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-013-0282-0`.

Munoz:2014:DPR

[2332] M. Teresa de Bustos Muñoz, Juan L. G. Guirao, and Jesús Vigo-Aguiar. Decomposition of pseudo-radioactive chemical products with a mathematical approach. *Journal of Mathematical Chemistry*, 52(4):1059–1065,

April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-013-0285-x.

Ray:2014:CAV

[2333] S. Saha Ray and A. K. Gupta. Comparative analysis of variational iteration method and Haar wavelet method for the numerical solutions of Burgers–Huxley and Huxley equations. *Journal of Mathematical Chemistry*, 52(4):1066–1080, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0327-z.

Liu:2014:NEP

[2334] Shiwei Liu, Juan Zheng, and Yonglei Fang. A new embedded 5(3) pair of modified Runge–Kutta–Nyström methods for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 52 (4):1081–1098, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0328-y.

Singh:2014:ASS

[2335] Randhir Singh, Jitendra Kumar, and Gnaneshwar Nelakanti. Approximate series solution of fourth-order boundary value problems using decomposition method with Green's function. *Journal of Mathematical Chemistry*, 52(4):1099–1118, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0329-x.

Miraboutalebi:2014:SDS

[2336] S. Miraboutalebi and L. Rajaei. Solutions of N-dimensional Schrödinger equation with Morse potential via Laplace transforms. *Journal of Mathematical Chemistry*, 52(4):1119–1128, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0330-4.

Delgado:2014:SAK

[2337] Víctor Delgado. An stable approach to a kind of problems involving the inversion of a Volterra integral equation of the first kind: application to X-ray fluorescence analysis. *Journal of Mathematical Chemistry*, 52 (4):1129–1136, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0331-3.

Simpao:2014:RWG

[2338] Valentino A. Simpao. Real wavefunction from generalised Hamiltonian Schrödinger equation in quantum phase space via HOA (Heaviside Operational Ansatz): exact analytical results. *Journal of Mathematical Chemistry*, 52(4):1137–1155, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0332-2`.

Li:2014:AAM

[2339] Zhenquan Li. Accuracy analysis of a mesh refinement method using benchmarks of 2-D lid-driven cavity flows and finer meshes. *Journal of Mathematical Chemistry*, 52(4):1156–1170, April 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0334-0`.

Toropova:2014:ODT

[2340] Alla P. Toropova, Andrey A. Toropov, Valentin O. Kudyshkin, Danuta Leszczynska, and Jerzy Leszczynski. Optimal descriptors as a tool to predict the thermal decomposition of polymers. *Journal of Mathematical Chemistry*, 52(5):1171–1181, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0323-3`.

Alvarado-Soto:2014:ASO

[2341] Leonor Alvarado-Soto, Luis Alvarez-Thon, and Rodrigo Ramirez-Tagle. Aspects of spin-orbit effects in compounds containing heavy elements. *Journal of Mathematical Chemistry*, 52(5):1182–1190, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0314-4`.

Liu:2014:MAC

[2342] Ying Liu, Michael G. B. Drew, and Yue Liu. A mathematical approach to chemical equilibrium theory for gaseous systems — III: Q_p, Q_c, and Q_x. *Journal of Mathematical Chemistry*, 52(5):1191–1200, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0306-4`.

Belkic:2014:SRD

[2343] Dzevad Belkić. Survival of radiation-damaged cells via mechanism of repair by pool molecules: the Lambert function as the exact analytical solution of coupled kinetic equations. *Journal of Mathematical Chemistry*, 52(5):1201–1252, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0307-3.

Belkic:2014:RIC

[2344] Dzevad Belkić. Repair of irradiated cells by Michaelis–Menten enzyme catalysis: the Lambert function for integrated rate equations in description of surviving fractions. *Journal of Mathematical Chemistry*, 52(5): 1253–1291, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0308-2.

Nalewajski:2014:QID

[2345] Roman F. Nalewajski. Quantum information descriptors and communications in molecules. *Journal of Mathematical Chemistry*, 52(5): 1292–1323, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0311-7; http://link.springer.com/content/pdf/10.1007/s10910-014-0311-7.pdf.

Khuri:2014:VAC

[2346] S. A. Khuri and Abdul-Majid Wazwaz. A variational approach for a class of nonlocal elliptic boundary value problems. *Journal of Mathematical Chemistry*, 52(5):1324–1337, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0312-6.

Shobukhov:2014:ESS

[2347] Andrey V. Shobukhov and Dmitry S. Maximov. Exact steady state solutions in symmetrical Nernst–Planck–Poisson electrodiffusive models. *Journal of Mathematical Chemistry*, 52(5):1338–1349, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0313-5.

Skakauskas:2014:SMM

[2348] V. Skakauskas and P. Katauskis. Spillover in monomer-monomer reactions on supported catalysts: dynamic mean-field study. *Journal of Mathematical Chemistry*, 52(5):1350–1363, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0315-3.

Mikulski:2014:AAS

[2349] Damian Mikulski, Krzysztof Eder, and Jerzy Konarski. Approximate analytical solutions of the stationary radial Schrödinger equation with

new anharmonic potentials. *Journal of Mathematical Chemistry*, 52 (5):1364–1371, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0316-2; http://link.springer.com/content/pdf/10.1007/s10910-014-0316-2.pdf.

Toranzo:2014:FMN

[2350] I. V. Toranzo, J. S. Dehesa, and P. Sánchez-Moreno. Frequency moments, L_q norms and Rényi entropies of general hypergeometric polynomials. *Journal of Mathematical Chemistry*, 52(5):1372–1385, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0317-1.

Rudan:2014:PTA

[2351] János Rudan, Gábor Szederkényi, Katalin M. Hangos, and Tamás Péni. Polynomial time algorithms to determine weakly reversible realizations of chemical reaction networks. *Journal of Mathematical Chemistry*, 52 (5):1386–1404, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0318-0.

Roy:2014:RVS

[2352] Amlan K. Roy. Ro-vibrational spectroscopy of molecules represented by a Tietz–Hua oscillator potential. *Journal of Mathematical Chemistry*, 52 (5):1405–1413, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0319-z.

Pohjoranta:2014:MFP

[2353] Antti Pohjoranta and Robert Tenno. Microvia fill process model and control. *Journal of Mathematical Chemistry*, 52(5):1414–1440, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0320-6.

Zhang:2014:DAS

[2354] Tonghua Zhang, Zhenzhen Chen, and Maoan Han. Dynamical analysis of a stochastic model for cascaded continuous flow bioreactors. *Journal of Mathematical Chemistry*, 52(5):1441–1459, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0321-5.

Emelianenko:2014:ERC

[2355] Maria Emelianenko, Diego Torrejon, Matthew A. DeNardo, Annika K. Socolofsky, Alexander D. Ryabov, and Terrence J. Collins. Estimation of rate constants in nonlinear reactions involving chemical inactivation of oxidation catalysts. *Journal of Mathematical Chemistry*, 52 (5):1460–1476, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0322-4`.

Yang:2014:DSM

[2356] Ying Yang, Yanan Zhao, and Daqing Jiang. The dynamics of the stochastic multi-molecule biochemical reaction model. *Journal of Mathematical Chemistry*, 52(5):1477–1495, May 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0324-2`.

Bispo:2014:AST

[2357] Jose A. C. Bispo, Carlos F. S. Bonafe, Marília L. C. Silva, Ivo H. P. Andrade, and Giovani B. M. Carvalho. Applying structural transition theory to describe enzyme kinetics in heterogeneous systems. *Journal of Mathematical Chemistry*, 52(6):1497–1513, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0325-1`.

Fujita:2014:TAA

[2358] Shinsaku Fujita. Three aspects of an absolute configuration on the basis of the stereoisogram approach and revised terminology on related stereochemical concepts. *Journal of Mathematical Chemistry*, 52(6):1514–1534, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0326-0`.

Jiwari:2014:CMT

[2359] Ram Jiwari and Jinyun Yuan. A computational modeling of two dimensional reaction-diffusion Brusselator system arising in chemical processes. *Journal of Mathematical Chemistry*, 52(6):1535–1551, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0333-1`.

Mikulski:2014:SQM

[2360] Damian Mikulski, Krzysztof Eder, and Jerzy Konarski. The supersymmetric quantum mechanics theory and Darboux transformation for the

Morse oscillator with an approximate rotational term. *Journal of Mathematical Chemistry*, 52(6):1552–1562, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0335-z`.

Kaatz:2014:ITM

[2361] Forrest H. Kaatz and Adhemar Bultheel. Informational thermodynamic model for nanostructures. *Journal of Mathematical Chemistry*, 52(6):1563–1575, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0336-y`.

Fernandez:2014:BSC

[2362] Francisco M. Fernández. Bound states of a charged particle in the field of an electric quadrupole in two dimensions. *Journal of Mathematical Chemistry*, 52(6):1576–1580, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0337-x`.

Deng:2014:ESI

[2363] Kecai Deng and Jianguo Qian. Enumerating stereo-isomers of tree-like polyinositols. *Journal of Mathematical Chemistry*, 52(6):1581–1598, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0338-9`.

Boykin:2014:EIB

[2364] Timothy B. Boykin. Effective interactions and block diagonalization in quantum-mechanical problems. *Journal of Mathematical Chemistry*, 52(6):1599–1609, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0339-8`.

Mikulski:2014:AAD

[2365] Damian Mikulski, Krzysztof Eder, and Marcin Molski. The algebraic approach for the derivation of ladder operators and coherent states for the Goldman and Krivchenkov oscillator by the use of supersymmetric quantum mechanics. *Journal of Mathematical Chemistry*, 52(6):1610–1623, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0341-1; http://link.springer.com/content/pdf/10.1007/s10910-014-0341-1.pdf`.

Wirth:2014:RBE

[2366] Karl Wirth and André S. Dreiding. Relations between edge lengths, dihedral and solid angles in tetrahedra. *Journal of Mathematical Chemistry*, 52(6):1624–1638, June 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0342-0`.

Bhattacharyya:2014:RSO

[2367] Kamal Bhattacharyya. Restrictions on second order response properties of quantum states. *Journal of Mathematical Chemistry*, 52(7): 1639–1646, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0355-8`.

Garcia-Sevilla:2014:LCSa

[2368] Francisco Garcia-Sevilla, Manuela Garcia-Moreno, Maria D. Masia, Ricardo Gomez-Ladron de Guevara, Maria M. Garcia-Molina, Enrique Arribas, Milagros Molina-Alarcon, Maria L. Amo, and Ramon Varon. Linear compartmental systems. III. Application to enzymatic reactions. *Journal of Mathematical Chemistry*, 52(7):1647–1674, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0360-y`.

Garcia-Sevilla:2014:LCSb

[2369] Francisco Garcia-Sevilla, Manuela Garcia-Moreno, Maria D. Masia, Ricardo Gomez-Ladron de Guevara, Maria M. Garcia-Molina, Enrique Arribas, Milagros Molina-Alarcon, Maria L. Amo, and Ramon Varon. Linear compartmental systems. IV. A software, under MS-Windows, for obtaining the instantaneous species concentrations in enzyme systems. *Journal of Mathematical Chemistry*, 52(7):1675–1689, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0361-x`.

Simos:2014:NEH

[2370] T. E. Simos. A new explicit hybrid four-step method with vanished phase-lag and its derivatives. *Journal of Mathematical Chemistry*, 52(7): 1690–1716, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0343-z`.

Fujita:2014:SIEc

[2371] Shinsaku Fujita. Symmetry-itemized enumeration of RS-stereoisomers of allenes. I. The fixed-point matrix method of the USCI approach com-

bined with the stereoisogram approach. *Journal of Mathematical Chemistry*, 52(7):1717–1750, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0344-y`.

Fujita:2014:SIEd

[2372] Shinsaku Fujita. Symmetry-itemized enumeration of RS-stereoisomers of allenes: II-the partial-cycle-index method of the USCI approach combined with the stereoisogram approach. *Journal of Mathematical Chemistry*, 52(7):1751–1793, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0345-x`.

Alcoba:2014:SAF

[2373] Diego R. Alcoba, Gustavo E. Massaccesi, Ofelia B. Oña, Juan J. Torres-Vega, Luis Lain, and Alicia Torre. Symmetry-adapted formulation of the combined G-particle-hole hypervirial equation and Hermitian operator method. *Journal of Mathematical Chemistry*, 52(7):1794–1806, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0346-9`.

Liu:2014:RGG

[2374] Saihua Liu, Jianping Ou, and Youchuang Lin. On k-resonance of grid graphs on the plane, torus and cylinder. *Journal of Mathematical Chemistry*, 52(7):1807–1816, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0347-8`.

Sumetpipat:2014:CNN

[2375] Kanes Sumetpipat, Richard K. F. Lee, Barry J. Cox, James M. Hill, and Duangkamon Baowan. Carbon nanotori and nanotubes encapsulating carbon atomic-chains. *Journal of Mathematical Chemistry*, 52(7):1817–1830, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0348-7`.

Chu:2014:EAV

[2376] Rainer Kwang-Hua Chu. Effect of activation volume on the defect-induced anomalous electronic transport in $Rb_{0.8}Fe_2Se_2$. *Journal of Mathematical Chemistry*, 52(7):1831–1840, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0349-6`.

Lu:2014:SST

[2377] Fuliang Lu, Yajun Gong, and Houchun Zhou. The spectrum and spanning trees of polyominos on the torus. *Journal of Mathematical Chemistry*, 52(7):1841–1847, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0350-0`.

Carbo-Dorca:2014:MPQ

[2378] Ramon Carbó-Dorca. Multimolecular polyhedra and QSPR. *Journal of Mathematical Chemistry*, 52(7):1848–1856, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0351-z`.

Kuruoglu:2014:MVB

[2379] Zeki C. Kuruoglu. Multi-variate Bateman method for two-body scattering without partial-wave decomposition. *Journal of Mathematical Chemistry*, 52(7):1857–1869, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0352-y`.

Shokri:2014:TFH

[2380] Ali Shokri and Hosein Saadat. Trigonometrically fitted high-order predictor-corrector method with phase-lag of order infinity for the numerical solution of radial Schrödinger equation. *Journal of Mathematical Chemistry*, 52(7):1870–1894, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0353-x`.

Simos:2014:ELS

[2381] T. E. Simos. An explicit linear six-step method with vanished phase-lag and its first derivative. *Journal of Mathematical Chemistry*, 52(7):1895–1920, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0354-9`.

Nalewajski:2014:QIA

[2382] Roman F. Nalewajski. Quantum information approach to electronic equilibria: molecular fragments and non-equilibrium thermodynamic description. *Journal of Mathematical Chemistry*, 52(7):1921–1948, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0357-6; http://link.springer.com/content/pdf/10.1007/s10910-014-0357-6.pdf`.

Carbo-Dorca:2014:PIQ

[2383] Ramon Carbó-Dorca and Emili Besalú. A postulate involving quantum mechanical momentum in position space, density function expression of the kinetic energy and Heisenberg's uncertainty relation. *Journal of Mathematical Chemistry*, 52(7):1949–1967, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0358-5`.

Hutem:2014:ECF

[2384] Artit Hutem and Sutee Boonchui. Evaluation of correlation functions and wave-functions of the Gaussian random potentials by numerical shooting method. *Journal of Mathematical Chemistry*, 52(7):1968–1977, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0359-4`.

Petrov:2014:SCP

[2385] Dimitar Petrov. Spin correlation in Pr IV and Tm IV free ions. *Journal of Mathematical Chemistry*, 52(7):1978–1983, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0362-9`.

Cao:2014:WPA

[2386] Junfei Cao, Zaitang Huang, and Caibin Zeng. Weighted pseudo almost automorphic classical solutions and optimal mild solutions for fractional differential equations and application in fractional reaction-diffusion equations. *Journal of Mathematical Chemistry*, 52(7):1984–2012, August 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0373-6`.

Bucknum:2014:PCH

[2387] Michael J. Bucknum and Eduardo A. Castro. Preservation of C hexagons in the transformation of C allotropes. *Journal of Mathematical Chemistry*, 52(8):2013–2019, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0383-4`.

Ivanauskas:2014:MEP

[2388] Feliksas Ivanauskas, Albertas Malinauskas, and Liana Stonkiene. Modeling of electrocatalysis at polyaniline-modified electrodes: autoacceleration of the process by the reaction product. *Journal of Mathematical Chemistry*, 52(8):2020–2029, September 2014. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0366-5`.

Singh:2014:NET

[2389] Randhir Singh, Gnaneshwar Nelakanti, and Jitendra Kumar. A new efficient technique for solving two-point boundary value problems for integro-differential equations. *Journal of Mathematical Chemistry*, 52(8): 2030–2051, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0363-8`.

Li:2014:AHF

[2390] Genyuan Li and Herschel Rabitz. Analytical HDMR formulas for functions expressed as quadratic polynomials with a multivariate normal distribution. *Journal of Mathematical Chemistry*, 52(8):2052–2073, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0365-6`.

Feng:2014:PGA

[2391] Liqiang Feng, Hang Liu, and Xingjiang Liu. Polarized gating assisted generation of the ultrashort extreme-ultraviolet sources. *Journal of Mathematical Chemistry*, 52(8):2074–2086, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0367-4`.

Alolyan:2014:FEL

[2392] Ibraheem Alolyan and T. E. Simos. A family of explicit linear six-step methods with vanished phase-lag and its first derivative. *Journal of Mathematical Chemistry*, 52(8):2087–2118, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0364-7`.

Glasser:2014:QMS

[2393] M. L. Glasser. Quantum mechanics of a simulated trihydrogen dication. *Journal of Mathematical Chemistry*, 52(8):2119–2127, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0370-9`.

Fernandez:2014:HFT

[2394] Francisco M. Fernández. The Hellmann–Feynman theorem for statistical averages. *Journal of Mathematical Chemistry*, 52(8):2128–2132, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (elec-

tronic). URL http://link.springer.com/article/10.1007/s10910-014-0368-3.

Wazwaz:2014:CRE

[2395] Abdul-Majid Wazwaz. A coupled Ramani equation: multiple soliton solutions. *Journal of Mathematical Chemistry*, 52(8):2133–2140, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0372-7.

Thilagam:2014:EPQ

[2396] A. Thilagam. Exciton propagation via quantum walks based on non-Hermitian coin flip operations. *Journal of Mathematical Chemistry*, 52(8):2141–2160, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0369-2.

Ayvaz:2014:PEAa

[2397] Muzaffer Ayvaz and Metin Demiralp. Probabilistic evolution approach to the expectation value dynamics of quantum mechanical operators, part I: integral representation of Kronecker power series and multivariate Hausdorff moment problems. *Journal of Mathematical Chemistry*, 52(8): 2161–2182, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0371-8.

Lalik:2014:COS

[2398] Erwin Lalik. Chaos in oscillatory sorption of hydrogen in palladium. *Journal of Mathematical Chemistry*, 52(8):2183–2196, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0374-5; http://link.springer.com/content/pdf/10.1007/s10910-014-0374-5.pdf.

Peng:2014:SMT

[2399] Jiangtao Peng. Sparse matrix transform based weight updating in partial least squares regression. *Journal of Mathematical Chemistry*, 52(8):2197–2209, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0380-7.

Szabados:2014:LBF

[2400] Ágnes Szabados and Zsuzsanna Tóth. Löwdin's bracketing function revisited. *Journal of Mathematical Chemistry*, 52(8):2210–2221, Septem-

ber 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0379-0.

Jia:2014:SAP

[2401] Ji-Teng Jia and Qiong-Xiang Kong. A symbolic algorithm for periodic tridiagonal systems of equations. *Journal of Mathematical Chemistry*, 52(8):2222–2233, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0378-1.

Msmali:2014:QAN

[2402] Ahmed Hussein Msmali, Mark I. Nelson, and Maureen P. Edwards. Quadratic autocatalysis with non-linear decay. *Journal of Mathematical Chemistry*, 52(8):2234–2258, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0382-5.

Banerjee:2014:FFP

[2403] Kinshuk Banerjee. On the flux-force partitioning and non-equilibrium thermodynamics near a steady state. *Journal of Mathematical Chemistry*, 52(8):2259–2270, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0385-2.

Palmeira:2014:DCD

[2404] Tiago Palmeira and Mário N. Berberan-Santos. Distinctive characteristics of the decay function for phosphorescence in the presence of reabsorption. *Journal of Mathematical Chemistry*, 52(8):2271–2276, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0376-3.

Ray:2014:TDH

[2405] S. Saha Ray and A. K. Gupta. A two-dimensional Haar wavelet approach for the numerical simulations of time and space fractional Fokker–Planck equations in modelling of anomalous diffusion systems. *Journal of Mathematical Chemistry*, 52(8):2277–2293, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0384-3.

Ayvaz:2014:PEAb

[2406] Muzaffer Ayvaz and Metin Demiralp. Probabilistic evolution approach to the expectation value dynamics of quantum mechanical operators, part

II: the use of mathematical fluctuation theory. *Journal of Mathematical Chemistry*, 52(8):2294–2315, September 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0381-6`.

Mikulski:2014:FIE

[2407] Damian Mikulski, Krzysztof Eder, and Jerzy Konarski. Fredholm integral equation for the perturbation theory in quantum mechanics. *Journal of Mathematical Chemistry*, 52(9):2317–2321, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0387-0; http://link.springer.com/content/pdf/10.1007/s10910-014-0387-0.pdf`.

Fernandez:2014:CEL

[2408] Francisco M. Fernández. On the crossing of the energy levels of a parameter-dependent quantum-mechanical Hamiltonian. *Journal of Mathematical Chemistry*, 52(9):2322–2329, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0386-1`.

Gutman:2014:FML

[2409] Ivan Gutman. Frank model with limited resources. *Journal of Mathematical Chemistry*, 52(9):2330–2333, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0388-z`.

Alolyan:2014:HTF

[2410] Ibraheem Alolyan and T. E. Simos. A hybrid type four-step method with vanished phase-lag and its first, second and third derivatives for each level for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 52(9):2334–2379, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0375-4`.

Duan:2014:MDD

[2411] Jin-Wei Duan, Wei Li, Xiao-Wei Li, Guang Hu, and Wen-Yuan Qiu. Molecular design of DNA polyhedra based on genus. *Journal of Mathematical Chemistry*, 52(9):2380–2394, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0389-y`.

Arteca:2014:CQM

[2412] Gustavo A. Arteca, Laura Laverdure, and O. Tapia. Constructing quantum mechanical models from diabatic schemes: external field modulation of effective energy barriers for bond breaking/formation processes. *Journal of Mathematical Chemistry*, 52(9):2395–2410, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0377-2`.

Strekalov:2014:EAS

[2413] Mikhail L. Strekalov. An exact analytical solution to the master equation for the vibration-dissociation process of Morse oscillators. *Journal of Mathematical Chemistry*, 52(9):2411–2422, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0391-4`.

Graves:2014:CSN

[2414] Christina Graves and Stephen J. Graves. Counting symmetric and near-symmetric fullerene patches. *Journal of Mathematical Chemistry*, 52(9): 2423–2441, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0393-2`.

Masia:2014:AFM

[2415] Maria D. Masia, Manuela Garcia-Moreno, Francisco Garcia-Sevilla, Julio Escribano, Milagros Molina-Alarcon, Maria L. Amo-Saus, Enrique Arribas, and Ramon Varon. Analysis of the fractional modification of the monocyclic enzyme cascades, defined in an alternative way involving the two forms of the modified protein. *Journal of Mathematical Chemistry*, 52(9):2442–2458, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0392-3`.

Sharma:2014:AAD

[2416] Manju Sharma, Aditya Kaushik, and Chenglin Li. Analytic approximation to delayed convection dominated systems through transforms. *Journal of Mathematical Chemistry*, 52(9):2459–2474, October 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0394-1`.

DellAcqua:2014:AUA

[2417] Guido Dell'Acqua and Alberto Maria Bersani. On the appropriate use of asymptotic expansions in enzyme kinetics. *Journal of Mathematical*

Chemistry, 52(10):2475–2481, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0403-4`.

Choi:2014:ESW

[2418] Jin Hyuk Choi, Hyunsoo Kim, and Rathinasamy Sakthivel. Exact solution of the Wick-type stochastic fractional coupled KdV equations. *Journal of Mathematical Chemistry*, 52(10):2482–2493, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0406-1`.

Li:2014:SMT

[2419] Ronald Li, Robert A. Van Gorder, Kristina Mallory, and Kuppalapalle Vajravelu. Solution method for the transformed time-dependent Michaelis–Menten enzymatic reaction model. *Journal of Mathematical Chemistry*, 52(10):2494–2506, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0397-y`.

Chen:2014:TCR

[2420] Shaojie Chen, Xingye Zhang, Zhiyang Liu, and Ziyi Ge. Theoretical calculation on relationship between molecular structure and band gap of benzo[1,2-b:4,5-b']dithiophene based homopolymer. *Journal of Mathematical Chemistry*, 52(10):2507–2519, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0390-5`.

Cioslowski:2014:ESE

[2421] Jerzy Cioslowski and Joanna Albin. Electrostatic self-energies of discrete charge distributions on Jordan curves. *Journal of Mathematical Chemistry*, 52(10):2520–2531, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0395-0; http://link.springer.com/content/pdf/10.1007/s10910-014-0395-0.pdf`.

Yang:2014:DSL

[2422] Ying Yang and Daqing Jiang. Dynamics of the stochastic low concentration trimolecular chemical reaction model. *Journal of Mathematical Chemistry*, 52(10):2532–2545, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0398-x`.

Ozay:2014:REM

[2423] Evrim Korkmaz Özay and Metin Demiralp. Reductive enhanced multivariance product representation for multi-way arrays. *Journal of Mathematical Chemistry*, 52(10):2546–2558, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0396-z`.

Du:2014:DDE

[2424] Jian-Fen Du, Ping Guo, and Chun-Sheng Jia. D-dimensional energies for scandium monoiodide. *Journal of Mathematical Chemistry*, 52(10):2559–2569, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0399-9`.

Wu:2014:BBL

[2425] Xiaoqin P. Wu and Matthewos Eshete. Bautin bifurcation for the Lengyel–Epstein system. *Journal of Mathematical Chemistry*, 52(10):2570–2580, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0401-6`.

Laestadius:2014:KST

[2426] Andre Laestadius. Kohn–Sham theory in the presence of magnetic field. *Journal of Mathematical Chemistry*, 52(10):2581–2595, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0400-7`.

Goeke:2014:CAQ

[2427] Alexandra Goeke and Sebastian Walcher. A constructive approach to quasi-steady state reductions. *Journal of Mathematical Chemistry*, 52(10):2596–2626, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0402-5`.

Ugurlu:2014:RCC

[2428] Ekin Ugurlu and Elgiz Bairamov. On the rate of the convergence of the characteristic values of an integral operator associated with a dissipative fourth order differential operator in lim-4 case with finite transmission conditions. *Journal of Mathematical Chemistry*, 52(10):2627–2644, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0404-3`.

Roy:2014:GES

[2429] Amlan K. Roy. Ground and excited states of spherically symmetric potentials through an imaginary-time evolution method: application to spiked harmonic oscillators. *Journal of Mathematical Chemistry*, 52(10): 2645–2662, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0407-0`.

Wallace:2014:ESH

[2430] Rodrick Wallace. Extending Swerdlow's hypothesis: statistical models of mitochondrial deterioration and aging. *Journal of Mathematical Chemistry*, 52(10):2663–2679, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0418-x`.

Belkic:2014:PON

[2431] Dzevad Belkić and Karen Belkić. Padé optimization of noise-corrupted magnetic resonance spectroscopic time signals from fibroadenoma of the breast. *Journal of Mathematical Chemistry*, 52(10):2680–2713, November 2014. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0411-4`.

Nalewajski:2015:EDQ

[2432] Roman F. Nalewajski. Entropic descriptors of quantum communications in molecules. *Journal of Mathematical Chemistry*, 53(1):1–28, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0405-2; http://link.springer.com/content/pdf/10.1007/s10910-014-0405-2.pdf`.

Baowan:2015:QSB

[2433] Duangkamon Baowan and Volkhard Helms. Quantitative study of BSA coating silica nanoparticle. *Journal of Mathematical Chemistry*, 53(1): 29–40, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0408-z`.

Bofill:2015:SRM

[2434] Josep Maria Bofill, Wolfgang Quapp, and Efrem Bernuz. Some remarks on the model of the extended gentlest ascent dynamics. *Journal of Mathematical Chemistry*, 53(1):41–57, January 2015. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0409-y.

Cassam-Chenai:2015:FAC

[2435] Patrick Cassam-Chenaï, Guillaume Dhont, and Frédéric Patras. A fast algorithm for the construction of integrity bases associated to symmetry-adapted polynomial representations: application to tetrahedral XY_4 molecules. *Journal of Mathematical Chemistry*, 53(1):58–85, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0410-5.

Toth:2015:SAC

[2436] János Tóth, Attila László Nagy, and István Gyula Zsély. Structural analysis of combustion mechanisms. *Journal of Mathematical Chemistry*, 53(1):86–110, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0412-3.

Al-Zarka:2015:TBR

[2437] Aya Al-Zarka, Afnan Alagha, and S. Timoshin. Transient behaviour in RDA systems of the Schnakenberg type. *Journal of Mathematical Chemistry*, 53(1):111–127, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0413-2; http://link.springer.com/content/pdf/10.1007/s10910-014-0413-2.pdf.

Hua:2015:ITB

[2438] Wei Hua, Yan Lyu, and Xue Shen Liu. Interference of two Bose–Einstein condensates with varying initial conditions. *Journal of Mathematical Chemistry*, 53(1):128–136, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0414-1.

Mukherjee:2015:SAB

[2439] Neetik Mukherjee. A simulated annealing based study of the effect of Gaussian perturbation in quartic oscillator and quadratic double well potentials. *Journal of Mathematical Chemistry*, 53(1):137–150, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0415-0.

Zhou:2015:FPT

[2440] Wenjin Zhou and Allison M. Rossetto. Finding protein thermostability and spin-coupling constant using Bayesian statistics. *Journal of Mathematical Chemistry*, 53(1):151–161, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0416-z`. See erratum [2441].

Zhou:2015:EFP

[2441] Wenjin Zhou and Allison M. Rossetto. Erratum to: Finding protein thermostability and spin-coupling constant using Bayesian statistics. *Journal of Mathematical Chemistry*, 53(1):162, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0443-9; http://link.springer.com/content/pdf/10.1007/s10910-014-0443-9.pdf`. See [2440].

Tikhonov:2015:QAP

[2442] Nikolay A. Tikhonov and Gleb B. Sidelnikov. Quantitative analysis of physical factors that determine the behavior of activity coefficients of electrolytes. II. Dependence on temperature. *Journal of Mathematical Chemistry*, 53(1):163–170, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0417-y`.

Carbo-Dorca:2015:QPD

[2443] Ramon Carbó-Dorca. Quantum polyhedra, definitions, statistics and the construction of a collective quantum similarity index. *Journal of Mathematical Chemistry*, 53(1):171–182, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0419-9`.

Baas:2015:STL

[2444] Nils A. Baas, Nadrian C. Seeman, and Andrew Stacey. Synthesising topological links. *Journal of Mathematical Chemistry*, 53(1):183–199, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0420-3`.

Chung:2015:MDT

[2445] Won Sang Chung. Modified q-deformed Tamm–Dancoff oscillators as a model for vibrations of polyatomic molecule. *Journal of Mathematical*

Chemistry, 53(1):200–206, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0421-2`.

Quadras:2015:DCC

[2446] Jasintha Quadras, A. Sajiya Merlin Mahizl, Indra Rajasingh, and R. Sundara Rajan. Domination in certain chemical graphs. *Journal of Mathematical Chemistry*, 53(1):207–219, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0422-1`.

Gubernov:2015:FTI

[2447] Vladimir Vladimirovich Gubernov and Jong Soo Kim. The fast-time instability map of Liñán's diffusion-flame regime. *Journal of Mathematical Chemistry*, 53(1):220–235, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0423-0`.

Fernandez:2015:EDS

[2448] Francisco M. Fernández, Diego R. Alcoba, Ofelia B. Oña, Alicia Torre, and Luis Lain. Electronic densities in systems with fractionally charged nuclei: a symmetry breaking study. *Journal of Mathematical Chemistry*, 53(1):236–249, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0424-z`.

Michael:2015:VCA

[2449] J. Robert Michael and Tibor Koritsanszky. Validation of convolution approximation to the thermal-average electron density. *Journal of Mathematical Chemistry*, 53(1):250–259, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0425-y`.

Fujita:2015:STMa

[2450] Shinsaku Fujita. Stereoisograms for three-membered heterocycles: I. Symmetry-itemized enumeration of oxiranes under an RS-stereoisomeric group. *Journal of Mathematical Chemistry*, 53(1):260–304, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0426-x`.

Fujita:2015:STMb

[2451] Shinsaku Fujita. Stereoisograms for three-membered heterocycles: II. Chirality, RS-stereogenicity, and ortho-stereogenicity on the basis of the

proligand-promolecule model. *Journal of Mathematical Chemistry*, 53 (1):305–352, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0427-9`.

Fujita:2015:STMc

[2452] Shinsaku Fujita. Stereoisograms for three-membered heterocycles: III. R/S-stereodescriptors for characterizing the RS-stereogenic aspect of absolute configuration. *Journal of Mathematical Chemistry*, 53(1):353–373, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0428-8`.

Assemat:2015:CEF

[2453] E. Assémat, T. Chambrion, and D. Sugny. On the control by electromagnetic fields of quantum systems with infinite dimensional Hilbert space. *Journal of Mathematical Chemistry*, 53(1):374–385, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0429-7`.

Li:2015:ERR

[2454] Cong Li, Yunchao Wu, and Zheng Chen. Effects of reaction reversibility on ignition and flame propagation. *Journal of Mathematical Chemistry*, 53(1):386–401, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0430-1`.

Simos:2015:NEF

[2455] T. E. Simos. A new explicit four-step method with vanished phase-lag and its first and second derivatives. *Journal of Mathematical Chemistry*, 53(1):402–429, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0431-0`.

Cordero:2015:SNP

[2456] Alicia Cordero, Javier G. Maimó, Juan R. Torregrosa, and María P. Vassileva. Solving nonlinear problems by Ostrowski–Chun type parametric families. *Journal of Mathematical Chemistry*, 53(1):430–449, January 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0432-z`. See erratum [2501].

Martinez-Araya:2015:WDD

[2457] Jorge Ignacio Martínez-Araya. Why is the dual descriptor a more accurate local reactivity descriptor than Fukui functions? *Journal of Mathematical Chemistry*, 53(2):451–465, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0437-7`.

Thilagam:2015:NLH

[2458] A. Thilagam. Natural light harvesting systems: unraveling the quantum puzzles. *Journal of Mathematical Chemistry*, 53(2):466–494, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0442-x`.

Turulski:2015:DGFa

[2459] Jan Turulski. Dimension of the Gibbs function topological manifold: 1. Graph representation of the thermodynamic equilibrium state. *Journal of Mathematical Chemistry*, 53(2):495–513, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0439-5`. See erratum [2460].

Turulski:2015:EDGa

[2460] Jan Turulski. Erratum to: Dimension of the Gibbs function topological manifold: 1. Graph representation of the thermodynamic equilibrium state. *Journal of Mathematical Chemistry*, 53(2):514–516, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0471-5; http://link.springer.com/content/pdf/10.1007/s10910-014-0471-5.pdf`. See [2459].

Turulski:2015:DGFb

[2461] Jan Turulski. Dimension of the Gibbs function topological manifold: 2. Thermodynamically stable binary quasicrystals: Reality or artefact? *Journal of Mathematical Chemistry*, 53(2):517–526, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0438-6`. See erratum [2462].

Turulski:2015:EDGb

[2462] Jan Turulski. Erratum to: Dimension of the Gibbs function topological manifold: 2. Thermodynamically stable binary quasicrystals: Reality

or artefact? *Journal of Mathematical Chemistry*, 53(2):527, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0470-6; http://link.springer.com/content/pdf/10.1007/s10910-014-0470-6.pdf`. See [2461].

Akimov:2015:ASC

[2463] Alexey V. Akimov and Oleg V. Prezhdo. Analysis of self-consistent extended Hückel theory (SC-EHT): a new look at the old method. *Journal of Mathematical Chemistry*, 53(2):528–550, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0433-y`.

Chen:2015:WTS

[2464] Shu-Chuan Chen, Dan M. Hayden, and Stanley S. Young. The wavelet transforms and statistical models for near infrared spectra analysis. *Journal of Mathematical Chemistry*, 53(2):551–572, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0434-x`.

Dehesa:2015:ECA

[2465] J. S. Dehesa, A. Guerrero, and P. Sánchez-Moreno. Entropy and complexity analysis of the D-dimensional rigid rotator and hyperspherical harmonics. *Journal of Mathematical Chemistry*, 53(2):573–589, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0435-9`.

Carbo-Dorca:2015:CRP

[2466] Ramon Carbó-Dorca. Coulomb repulsion, point-like nuclear charges, Dirac paradox, soft nuclear charge density and hypermultiplet nuclear repulsion. *Journal of Mathematical Chemistry*, 53(2):590–603, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0436-8`.

Skakauskas:2015:MDD

[2467] V. Skakauskas and P. Katauskis. Modelling dimer-dimer reactions on supported catalysts. *Journal of Mathematical Chemistry*, 53(2):604–617, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0440-z`.

Das:2015:LTA

[2468] Tapas Das. A Laplace transform approach to find the exact solution of the N-dimensional Schrödinger equation with Mie-type potentials and construction of ladder operators. *Journal of Mathematical Chemistry*, 53 (2):618–628, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0444-8`.

Paldus:2015:CSL

[2469] Josef Paldus, Tokuei Sako, and Geerd H. F. Diercksen. On the cluster structure of linear-chain fermionic wave functions. *Journal of Mathematical Chemistry*, 53(2):629–650, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0445-7`.

Sabelfeld:2015:SMF

[2470] Karl K. Sabelfeld, Oliver Brandt, and Vladimir M. Kaganer. Stochastic model for the fluctuation-limited reaction-diffusion kinetics in inhomogeneous media based on the nonlinear Smoluchowski equations. *Journal of Mathematical Chemistry*, 53(2):651–669, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0446-6`.

Verma:2015:SNT

[2471] Amit K. Verma and Mandeep Singh. Singular nonlinear three point BVPs arising in thermal explosion in a cylindrical reactor. *Journal of Mathematical Chemistry*, 53(2):670–684, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0447-5`.

Alolyan:2015:PCE

[2472] Ibraheem Alolyan and T. E. Simos. A predictor-corrector explicit four-step method with vanished phase-lag and its first, second and third derivatives for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 53(2):685–717, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0449-3`.

Donovan:2015:SAA

[2473] A. Donovan and H. Rabitz. Systematically altering the apparent topology of constrained quantum control landscapes. *Journal of Mathematical Chemistry*, 53(2):718–736, February 2015. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0453-7.

Powers:2015:SAC

[2474] Joseph M. Powers, Samuel Paolucci, Joshua D. Mengers, and Ashraf N. Al-Khateeb. Slow attractive canonical invariant manifolds for reactive systems. *Journal of Mathematical Chemistry*, 53(2):737–766, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0454-6.

Singh:2015:EAS

[2475] Randhir Singh and Abdul-Majid Wazwaz. An efficient approach for solving second-order nonlinear differential equation with Neumann boundary conditions. *Journal of Mathematical Chemistry*, 53(2):767–790, February 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0455-5.

Vigo-Aguiar:2015:MCT

[2476] J. Vigo-Aguiar and Higinio Ramos. Mathematical and computational tools in chemistry: CMMSE-2014. *Journal of Mathematical Chemistry*, 53(3):791–793, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0475-9; http://link.springer.com/content/pdf/10.1007/s10910-015-0475-9.pdf.

Garcia-Martinez:2015:EAS

[2477] J. M. García-Martínez, E. M. Garzón, J. M. Cecilia, H. Pérez-Sánchez, and P. M. Ortigosa. An efficient approach for solving the HP protein folding problem based on UEGO. *Journal of Mathematical Chemistry*, 53(3):794–806, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0459-1.

Campos:2015:BFC

[2478] B. Campos, A. Cordero, J. R. Torregrosa, and P. Vindel. Behaviour of fixed and critical points of the (α, c)-family of iterative methods. *Journal of Mathematical Chemistry*, 53(3):807–827, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-014-0465-3.

Calvo-Jurado:2015:HSB

[2479] Carmen Calvo-Jurado and William J. Parnell. Hashin–Shtrikman bounds on the effective thermal conductivity of a transversely isotropic two-phase composite material. *Journal of Mathematical Chemistry*, 53(3): 828–843, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0452-8`.

Lal:2015:SAM

[2480] Rajnesh Lal and Zhenquan Li. Sensitivity analysis of a mesh refinement method using the numerical solutions of 2D lid-driven cavity flow. *Journal of Mathematical Chemistry*, 53(3):844–867, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0461-7`.

Kouibia:2015:VSM

[2481] A. Kouibia, M. Pasadas, Z. Belhaj, and A. Hananel. The variational spline method for solving Troesch's problem. *Journal of Mathematical Chemistry*, 53(3):868–879, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0462-6`.

Hueso:2015:DMR

[2482] José L. Hueso, Eulalia Martínez, and Carles Teruel. Determination of multiple roots of nonlinear equations and applications. *Journal of Mathematical Chemistry*, 53(3):880–892, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0460-8`.

Cordero:2015:NFO

[2483] Alicia Cordero, Licheng Feng, Alberto Magreñán, and Juan R. Torregrosa. A new fourth-order family for solving nonlinear problems and its dynamics. *Journal of Mathematical Chemistry*, 53(3):893–910, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0464-4`.

Pekmen:2015:DSN

[2484] B. Pekmen and M. Tezer-Sezgin. DRBEM solution of natural convective heat transfer with a non-Darcy model in a porous medium. *Journal of Mathematical Chemistry*, 53(3):911–924, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0448-4`.

Bayon:2015:SAL

[2485] L. Bayón, J. A. Otero, M. M. Ruiz, P. M. Suárez, and C. Tasis. Sensitivity analysis of a linear and unbranched chemical process with n steps. *Journal of Mathematical Chemistry*, 53(3):925–940, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0458-2`.

Rosa:2015:CLG

[2486] M. Rosa, M. S. Bruzón, and M. L. Gandarias. A conservation law for a generalized chemical Fisher equation. *Journal of Mathematical Chemistry*, 53(3):941–948, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0451-9`.

delaRosa:2015:SMH

[2487] R. de la Rosa, M. L. Gandarias, and M. S. Bruzón. A study for the microwave heating of some chemical reactions through Lie symmetries and conservation laws. *Journal of Mathematical Chemistry*, 53 (3):949–957, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0450-x`.

Morgado:2015:NMT

[2488] L. F. Morgado and M. L. Morgado. Numerical modelling transient current in the time-of-flight experiment with time-fractional advection-diffusion equations. *Journal of Mathematical Chemistry*, 53(3):958–973, March 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0463-5`.

Milani:2015:CFS

[2489] G. Milani, T. Hanel, R. Donetti, and F. Milani. A closed form solution for the vulcanization prediction of NR cured with sulphur and different accelerators. *Journal of Mathematical Chemistry*, 53(4):975–997, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0456-4`.

Fernandez:2015:PTM

[2490] Francisco M. Fernández. Perturbation theory by the moment method and point-group symmetry. *Journal of Mathematical Chemistry*, 53(4): 998–1009, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0457-3`.

Fujita:2015:CAG

[2491] Shinsaku Fujita. Combinatorial approach to group hierarchy for stereoskeletons of ligancy 4. *Journal of Mathematical Chemistry*, 53(4): 1010–1053, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0467-1`.

Duan:2015:SSC

[2492] Jun-Sheng Duan, Randolph Rach, and Abdul-Majid Wazwaz. Steady-state concentrations of carbon dioxide absorbed into phenyl glycidyl ether solutions by the Adomian decomposition method. *Journal of Mathematical Chemistry*, 53(4):1054–1067, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0469-z`.

Frolov:2015:PBH

[2493] Alexei M. Frolov and David M. Wardlaw. On the products of bipolar harmonics. *Journal of Mathematical Chemistry*, 53(4):1068–1079, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0466-2`.

Encinar:2015:RHA

[2494] Sonsoles Encinar, J. L. González-Hernández, M. Mar Canedo, and Diana Juanes. A robust hybrid algorithm (neural networks-AGDC) applied to non-isothermal kinetics of consecutive chemical reactions. *Journal of Mathematical Chemistry*, 53(4):1080–1104, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0472-z`.

Kwang-Hua:2015:CIF

[2495] Chu Rainer Kwang-Hua. Conductivities of ionic fluids in bismuth oxysulfates. *Journal of Mathematical Chemistry*, 53(4):1105–1112, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0441-y`.

Fatoorehchi:2015:CTC

[2496] H. Fatoorehchi, I. Gutman, and H. Abolghasemi. A combined technique for computation of energy-effect of cycles in conjugated molecules. *Journal of Mathematical Chemistry*, 53(4):1113–1125, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0473-y`.

Nalewajski:2015:REI

[2497] Roman F. Nalewajski. Resultant entropy/information, phase/entropy continuity and bond multiplicities in degenerate electronic states. *Journal of Mathematical Chemistry*, 53(4):1126–1161, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-014-0468-0; http://link.springer.com/content/pdf/10.1007/s10910-014-0468-0.pdf`.

Bira:2015:ESM

[2498] B. Bira and T. Raja Sekhar. Exact solutions to magnetogasdynamic equations in Lagrangian coordinates. *Journal of Mathematical Chemistry*, 53(4):1162–1171, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0476-8`.

Lente:2015:KIC

[2499] Gábor Lente. Kinetics of irreversible consecutive processes with first order second steps: analytical solutions. *Journal of Mathematical Chemistry*, 53(4):1172–1183, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0477-7`.

Furtula:2015:FTI

[2500] Boris Furtula and Ivan Gutman. A forgotten topological index. *Journal of Mathematical Chemistry*, 53(4):1184–1190, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0480-z`.

Cordero:2015:ESN

[2501] Alicia Cordero, Javier G. Maimó, Juan R. Torregrosa, and María P. Vassileva. Erratum to: Solving nonlinear problems by Ostrowski–Chun type parametric families. *Journal of Mathematical Chemistry*, 53(4):1191–1192, April 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0474-x; http://link.springer.com/content/pdf/10.1007/s10910-015-0474-x.pdf`. See [2456].

Fiordalis:2015:CPC

[2502] Andrew Fiordalis and Jerry Meldon. Concentration profile curvature for diffusion processes with simultaneous irreversible reaction. *Journal of Mathematical Chemistry*, 53(5):1193–1194, May

2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-015-0486-6; http://link.springer.com/article/10.1007/s10910-015-0486-6.

Carmona:2015:KIP

[2503] A. Carmona, A. M. Encinas, and M. Mitjana. Kirchhoff index of periodic linear chains. *Journal of Mathematical Chemistry*, 53(5):1195–1206, May 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0478-6.

Berberan-Santos:2015:PVL

[2504] Mário N. Berberan-Santos. Probabilistic view of the luminescence phasor plot and description of the universal semicircle as the sum of two spiraling curves. *Journal of Mathematical Chemistry*, 53(5):1207–1219, May 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0481-y.

Liu:2015:TEC

[2505] Jinxing Liu, Tianxiu Lu, and Risong Li. Topological entropy and $\mathcal{P}$-chaos of a coupled lattice system with non-zero coupling constant related with Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 53 (5):1220–1226, May 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0482-x.

Mackevicius:2015:CMS

[2506] Mazvydas Mackevicius, Feliksas Ivanauskas, Aivaras Kareiva, Vigirdas Mackevicius, and Andrius Stanulis. Computer modeling of synthesis of strontium stannates at high temperatures. *Journal of Mathematical Chemistry*, 53(5):1227–1238, May 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0483-9.

Mu:2015:RKT

[2507] Kenan Mu and T. E. Simos. A Runge–Kutta type implicit high algebraic order two-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of coupled differential equations arising from the Schrödinger equation. *Journal of Mathematical Chemistry*, 53(5):1239–1256, May 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0484-8.

Baricz:2015:BJI

[2508] Árpád Baricz, Tibor K. Pogány, Saminathan Ponnusamy, and Imre Rudas. Bounds for Jaeger integrals. *Journal of Mathematical Chemistry*, 53(5):1257–1273, May 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0485-7`.

Nagy:2015:ITA

[2509] I. Nagy and M. L. Glasser. Information-theoretic aspects of friction in the quantum mechanics of an interacting two-electron harmonic atom. *Journal of Mathematical Chemistry*, 53(5):1274–1279, May 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0487-5`.

Chan:2015:MMS

[2510] Yue Chan. Mathematical modeling and simulations on massive hydrogen yield using functionalized nanomaterials. *Journal of Mathematical Chemistry*, 53(5):1280–1293, May 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0488-4`.

Ning:2015:LCC

[2511] Hang Ning and T. E. Simos. A low computational cost eight algebraic order hybrid method with vanished phase-lag and its first, second, third and fourth derivatives for the approximate solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 53(6):1295–1312, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0489-3`.

Strekalov:2015:TDC

[2512] M. L. Strekalov. Time-dependent concentrations of reagents and products involved in the dissociation-recombination process. *Journal of Mathematical Chemistry*, 53(6):1313–1324, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0490-x`.

Falaye:2015:SSS

[2513] Babatunde J. Falaye, Sameer M. Ikhdair, and Majid Hamzavi. Spectroscopic study of some diatomic molecules via the proper quantization rule. *Journal of Mathematical Chemistry*, 53(6):1325–1350, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0491-9`.

Amore:2015:SES

[2514] Paolo Amore and Francisco M. Fernández. Small-energy series for one-dimensional quantum-mechanical models with non-symmetric potentials. *Journal of Mathematical Chemistry*, 53(6):1351–1362, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0492-8`.

Milani:2015:IRN

[2515] G. Milani and F. Milani. Iterative robust numerical procedure for the determination of kinetic constants in Han's model for NR cured with sulphur. *Journal of Mathematical Chemistry*, 53(6):1363–1379, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0493-7`.

CostaReis:2015:AVM

[2516] Martina Costa Reis. Application of variational methods in chemical thermodynamics: a study of the stability of chemical systems. *Journal of Mathematical Chemistry*, 53(6):1380–1392, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0494-6`.

Gan:2015:HBF

[2517] Wenzhen Gan, Canrong Tian, and Peng Zhu. Hopf bifurcation in a fractional diffusion food-limited models with feedback control. *Journal of Mathematical Chemistry*, 53(6):1393–1411, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0495-5`.

Banerjee:2015:DHV

[2518] Kinshuk Banerjee. Dynamic hysteresis in the velocity and dissipation of stochastic Michaelis–Menten kinetics. *Journal of Mathematical Chemistry*, 53(6):1412–1425, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0496-4`.

Frolov:2015:TPI

[2519] Alexei M. Frolov and David M. Wardlaw. Three-particle integrals with spherical Bessel and Neumann functions and photodetachment of the negatively charged hydrogen ions. *Journal of Mathematical Chemistry*, 53(6):1426–1444, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0497-3`.

vanderSchaft:2015:CDB

[2520] Arjan van der Schaft, Shodhan Rao, and Bayu Jayawardhana. Complex and detailed balancing of chemical reaction networks revisited. *Journal of Mathematical Chemistry*, 53(6):1445–1458, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0498-2; http://link.springer.com/content/pdf/10.1007/s10910-015-0498-2.pdf`.

Wang:2015:TEV

[2521] Xing-Jian Wang. Temperature effect on vertical detachment energy of bulk hydrated electron by dielectric continuum theory. *Journal of Mathematical Chemistry*, 53(6):1459–1469, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0499-1`.

Yang:2015:EFT

[2522] Yanping Yang, Ke Wu, and Yonglei Fang. Exponentially fitted TDRK pairs for the Schrödinger equation. *Journal of Mathematical Chemistry*, 53(6):1470–1487, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0500-z`.

Rosenfeld:2015:EGP

[2523] Vladimir R. Rosenfeld. Equivalent genomic (proteomic) sequences and semigroups. *Journal of Mathematical Chemistry*, 53(6):1488–1494, June 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0501-y`.

Alolyan:2015:HAOa

[2524] Ibraheem Alolyan and T. E. Simos. A high algebraic order predictor-corrector explicit method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of the Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 53(7):1495–1522, August 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0502-x`.

VanGorder:2015:SSS

[2525] Robert A. Van Gorder, Kalie Makowski, and Kristina Mallory. Self-similar solutions for the nonlinear dispersion of a chemical pollutant into

a river flow. *Journal of Mathematical Chemistry*, 53(7):1523–1536, August 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0503-9`.

Alajbegovic:2015:ZNZ

[2526] Hermina Alajbegović and Muharem Avdispahić. Zeta and normal zeta functions for a subclass of space groups. *Journal of Mathematical Chemistry*, 53(7):1537–1548, August 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0504-8`.

Nalewajski:2015:QID

[2527] Roman F. Nalewajski. Quantum information descriptors in position and momentum spaces. *Journal of Mathematical Chemistry*, 53(7):1549–1575, August 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0505-7; http://link.springer.com/content/pdf/10.1007/s10910-015-0505-7.pdf`.

Tarko:2015:CMS

[2528] Laszlo Tarko. Computation of the molecular shapes' similarity and diversity using USR method and General Shape Index. *Journal of Mathematical Chemistry*, 53(7):1576–1591, August 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0506-6`.

Oruc:2015:HWF

[2529] Ö. Oruç, F. Bulut, and A. Esen. A Haar wavelet-finite difference hybrid method for the numerical solution of the modified Burgers' equation. *Journal of Mathematical Chemistry*, 53(7):1592–1607, August 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0507-5`.

Thylwe:2015:AAP

[2530] K.-E. Thylwe. Applications of the amplitude-phase method to symmetric double-well potentials. *Journal of Mathematical Chemistry*, 53(7):1608–1616, August 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0508-4`.

Kong:2015:SPA

[2531] Qiong-Xiang Kong and Ji-Teng Jia. A structure-preserving algorithm for linear systems with circulant pentadiagonal coefficient matrices. *Jour-*

nal of Mathematical Chemistry, 53(7):1617–1633, August 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0509-3`.

Penfold:2015:EIM

[2532] Robert Penfold and Peter J. Wilde. Enumerating and indexing many-body intramolecular interactions: a graph theoretic approach. *Journal of Mathematical Chemistry*, 53(7):1634–1648, August 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0510-x; http://link.springer.com/content/pdf/10.1007/s10910-015-0510-x.pdf`.

Fernandez:2015:ACE

[2533] Francisco M. Fernández. About the crossing of the energy levels of a parameter-dependent quantum-mechanical Hamiltonian. *Journal of Mathematical Chemistry*, 53(8):1649–1650, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-015-0518-2; http://link.springer.com/article/10.1007/s10910-015-0518-2`.

Carbo-Dorca:2015:LSE

[2534] Ramon Carbó-Dorca. Least squares estimation of unknown molecular properties and quantum QSPR fundamental equation. *Journal of Mathematical Chemistry*, 53(8):1651–1656, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0521-7`.

Gabor:2015:RNR

[2535] Attila Gábor, Katalin M. Hangos, Julio R. Banga, and Gábor Szederkényi. Reaction network realizations of rational biochemical systems and their structural properties. *Journal of Mathematical Chemistry*, 53(8):1657–1686, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0511-9`.

Steel:2015:SSA

[2536] Mike Steel. Self-sustaining autocatalytic networks within open-ended reaction systems. *Journal of Mathematical Chemistry*, 53(8):1687–1701, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0512-8`.

Goedgebeur:2015:RGI

[2537] Jan Goedgebeur and Brendan D. McKay. Recursive generation of IPR fullerenes. *Journal of Mathematical Chemistry*, 53(8):1702–1724, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0513-7`.

Amovilli:2015:EPN

[2538] C. Amovilli and N. H. March. Electrostatic potentials at the nucleus for isoelectronic series of light atomic ions using the QMC method in relation to DFT. *Journal of Mathematical Chemistry*, 53(8):1725–1732, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0514-6`.

Banerjee:2015:CCI

[2539] Kinshuk Banerjee and Gautam Gangopadhyay. Characterization of conical intersection in a cis- trans isomerization through nonclassicality and entanglement. *Journal of Mathematical Chemistry*, 53(8):1733–1749, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0515-5`.

Carbo-Dorca:2015:IRPa

[2540] Ramon Carbó-Dorca. An isometric representation problem in quantum multimolecular polyhedra and similarity. *Journal of Mathematical Chemistry*, 53(8):1750–1758, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0516-4`.

Lente:2015:ASR

[2541] Gábor Lente. Analytical solutions for the rate equations of irreversible two-step consecutive processes with second order later steps. *Journal of Mathematical Chemistry*, 53(8):1759–1771, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0517-3`.

Barthel:2015:TEA

[2542] Senja Barthel and Dorothy Buck. Toroidal embeddings of abstractly planar graphs are knotted or linked. *Journal of Mathematical Chemistry*, 53(8):1772–1790, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0519-1;`

http://link.springer.com/content/pdf/10.1007/s10910-015-0519-1.pdf. See erratum [2784].

Jin:2015:TCT

[2543] Xian'an Jin and Xiao-Sheng Cheng. Topological chirality of a type of DNA and protein polyhedral links. *Journal of Mathematical Chemistry*, 53(8):1791–1807, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0520-8.

Alolyan:2015:ELC

[2544] Ibraheem Alolyan and T. E. Simos. Efficient low computational cost hybrid explicit four-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 53(8):1808–1834, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0522-6.

Liu:2015:MAC

[2545] Ying Liu, Yue Liu, and Michael G. B. Drew. A mathematical approach to chemical equilibrium theory for gaseous systems IV: a mathematical clarification of Le Chatelier's principle. *Journal of Mathematical Chemistry*, 53(8):1835–1870, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0523-5.

Rosenfeld:2015:SDP

[2546] Vladimir R. Rosenfeld. Some differential properties of Pólya's cycle indicators. *Journal of Mathematical Chemistry*, 53(8):1871–1875, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0524-4.

Carbo-Dorca:2015:IRPb

[2547] Ramon Carbó-Dorca. An isometric representation problem in quantum multimolecular polyhedra and similarity: (2) synisometry. *Journal of Mathematical Chemistry*, 53(8):1876–1884, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0525-3.

Li:2015:SNS

[2548] Genyuan Li, Roberto Rey de Castro, Xi Xing, and Herschel Rabitz. Sparse and nonnegative sparse D-MORPH regression. *Journal of Math-*

ematical Chemistry, 53(8):1885–1914, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0527-1`.

Alolyan:2015:HAOb

[2549] Ibraheem Alolyan and T. E. Simos. A high algebraic order multistage explicit four-step method with vanished phase-lag and its first, second, third, fourth and fifth derivatives for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 53(8):1915–1942, September 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0529-z`.

Tachibana:2015:GRS

[2550] Akitomo Tachibana. General relativistic symmetry of electron spin vorticity. *Journal of Mathematical Chemistry*, 53(9):1943–1965, October 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0528-0`.

Nalewajski:2015:PFD

[2551] Roman F. Nalewajski. On probability flow descriptors in position and momentum spaces. *Journal of Mathematical Chemistry*, 53(9):1966–1985, October 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0526-2; http://link.springer.com/content/pdf/10.1007/s10910-015-0526-2.pdf`.

Mikulski:2015:CGP

[2552] Damian Mikulski, Daniel Gasperowicz, and Jerzy Konarski. The construction of the Gilmore–Perelomov coherent states for the Kratzer–Fues anharmonic oscillator with the use of the algebraic approach. *Journal of Mathematical Chemistry*, 53(9):1986–1996, October 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0530-6`.

Arnrich:2015:SAI

[2553] Steffen Arnrich, Peter Bräuer, and Grit Kalies. Solving the adsorption integral equation with Langmuir-kernel and the influence of temperature on the stability of the solution. *Journal of Mathematical Chemistry*, 53(9):1997–2017, October 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0531-5`.

Mikulski:2015:ESS

[2554] Damian Mikulski, Jerzy Konarski, Krzysztof Eder, Marcin Molski, and Stanisław Kabaciński. Exact solution of the Schrödinger equation with a new expansion of anharmonic potential with the use of the supersymmetric quantum mechanics and factorization method. *Journal of Mathematical Chemistry*, 53(9):2018–2027, October 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0532-4`.

Cubillan:2015:NGL

[2555] Néstor Cubillán, Yovani Marrero-Ponce, Harold Ariza-Rico, Stephen J. Barigye, César R. García-Jacas, José R. Valdes-Martini, and Ysaías J. Alvarado. Novel global and local 3D atom-based linear descriptors of the Minkowski distance matrix: theory, diversity-variability analysis and QSPR applications. *Journal of Mathematical Chemistry*, 53(9): 2028–2064, October 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0533-3`.

Ismailov:2015:SFO

[2556] Z. I. Ismailov, B. O. Guler, and P. Ipek. Solvability of first order functional differential operators. *Journal of Mathematical Chemistry*, 53(9): 2065–2077, October 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0534-2`.

Brinkmann:2015:ENG

[2557] Gunnar Brinkmann, Dieter Mourisse, and Leanne Rylands. On the existence of nanojoins with given parameters. *Journal of Mathematical Chemistry*, 53(9):2078–2094, October 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0535-1`.

Rajaraman:2015:EWB

[2558] R. Rajaraman and G. Hariharan. An efficient wavelet based spectral method to singular boundary value problems. *Journal of Mathematical Chemistry*, 53(9):2095–2113, October 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0536-0`.

Li:2015:RPE

[2559] Risong Li and Yu Zhao. Remark on positive entropy of a coupled lattice system related with Belusov–Zhabotinskii reaction. *Journal of Math-*

ematical Chemistry, 53(10):2115–2119, November 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0538-y`.

Bucknum:2015:SCT

[2560] M. J. Bucknum and E. A. Castro. Structural chemistry and the transcendental numbers ϕ, e, and π. *Journal of Mathematical Chemistry*, 53(10):2120–2122, November 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0539-x`.

Skakauskas:2015:TMF

[2561] V. Skakauskas and P. Katauskis. Three mean-field models for bimolecular reactions proceeding on planar supported catalysts. *Journal of Mathematical Chemistry*, 53(10):2123–2136, November 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0542-2`.

Gubernov:2015:EDR

[2562] Vladimir V. Gubernov and Sergei S. Minaev. The effect of depletion of radicals on freely propagating hydrocarbon flames. *Journal of Mathematical Chemistry*, 53(10):2137–2154, November 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0543-1`.

Tunga:2015:WOH

[2563] Burcu Tunga and Metin Demiralp. Weight optimization in HDMR with perturbation expansion method. *Journal of Mathematical Chemistry*, 53(10):2155–2171, November 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0537-z`.

Frolov:2015:IFB

[2564] Alexei M. Frolov. On the interpolation formula for the bound state energies of atomic systems. *Journal of Mathematical Chemistry*, 53(10):2172–2183, November 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0544-0`.

Mezei:2015:UCV

[2565] Mihaly Mezei. Use of circular variance to quantify the deviation of a macromolecule from the spherical shape. *Journal of Mathematical Chemistry*, 53(10):2184–2190, November 2015. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0540-4.

Hui:2015:NFT

[2566] Fei Hui and T. E. Simos. A new family of two stage symmetric two-step methods with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 53(10):2191–2213, November 2015. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0545-z.

Joe-Wong:2016:CFO

[2567] Carlee Joe-Wong, Tak-San Ho, and Herschel Rabitz. On choosing the form of the objective functional for optimal control of molecules. *Journal of Mathematical Chemistry*, 54(1):1–9, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0558-7.

Fulop:2016:ISA

[2568] Ottilia Fülöp and Béla Barabás. Impact of the Soai-autocatalysis on natural sciences. *Journal of Mathematical Chemistry*, 54(1):10–17, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0573-8.

Jiang:2016:MFN

[2569] Xiaoyan Jiang and Heping Zhang. The maximum forcing number of cylindrical grid, toroidal 4–8 lattice and Klein bottle 4–8 lattice. *Journal of Mathematical Chemistry*, 54(1):18–32, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0541-3.

Kaatz:2016:DHC

[2570] Forrest H. Kaatz and Adhemar Bultheel. Dimensionality of hypercube clusters. *Journal of Mathematical Chemistry*, 54(1):33–43, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0546-y.

CostaReis:2016:NET

[2571] Martina Costa Reis, Maria de Fátima Brito Sousa, Celso Aparecido Bertran, and Adalberto Bono Maurizio Sacchi Bassi. Non-equilibrium thermodynamic model for calcium carbonate supersaturated solutions of high salinity. *Journal of Mathematical Chemistry*, 54(1):44–60, January

2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0547-x.

Carbo-Dorca:2016:SCV

[2572] Ramon Carbó-Dorca. A study on the centroid vector of a polyhedron. *Journal of Mathematical Chemistry*, 54(1):61–71, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0548-9.

Arimoto:2016:PAL

[2573] Shigeru Arimoto. Proof of the Asymptotic Linearity Theorem Extension Conjecture (ALTEC). *Journal of Mathematical Chemistry*, 54(1):72–84, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0549-8.

Tobias:2016:SAS

[2574] Roland Tóbiás and Gyula Tasi. Simple algebraic solutions to the kinetic problems of triangle, quadrangle and pentangle reactions. *Journal of Mathematical Chemistry*, 54(1):85–99, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0550-2.

Kwang-Hua:2016:FWB

[2575] Chu Rainer Kwang-Hua. Formation of weakly bound molecular complexes: $(^3\,\mathrm{He})_2$. *Journal of Mathematical Chemistry*, 54(1):100–108, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0551-1.

Kyurkchiev:2016:HDB

[2576] Nikolay Kyurkchiev and Svetoslav Markov. On the Hausdorff distance between the Heaviside step function and Verhulst logistic function. *Journal of Mathematical Chemistry*, 54(1):109–119, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0552-0.

Wu:2016:BTS

[2577] Hongxia Wu and Xiaoqin P. Wu. Bogdanov–Takens singularity for a system of reaction–diffusion equations. *Journal of Mathematical Chemistry*, 54(1):120–136, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0553-z.

Quapp:2016:CWU

[2578] Wolfgang Quapp. Can we understand the branching of reaction valleys for more than two degrees of freedom? *Journal of Mathematical Chemistry*, 54(1):137–148, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0554-y`.

Belkic:2016:HFP

[2579] Dzevad Belkić and Karen Belkić. How the fast Padé transform handles noise for MRS data from the ovary: importance for ovarian cancer diagnostics. *Journal of Mathematical Chemistry*, 54(1):149–185, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0555-x`.

Belkic:2016:MOM

[2580] Dzevad Belkić and Karen Belkić. Mathematically-optimized magnetic resonance spectroscopy in breast cancer diagnostics: implications for personalized cancer medicine. *Journal of Mathematical Chemistry*, 54(1):186–230, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0556-9`.

Singh:2016:ECT

[2581] Mandeep Singh and Amit K. Verma. An effective computational technique for a class of Lane–Emden equations. *Journal of Mathematical Chemistry*, 54(1):231–251, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0557-8`.

Wazwaz:2016:GSW

[2582] Abdul-Majid Wazwaz. Gaussian solitary waves for the logarithmic-BBM and the logarithmic-TRLW equations. *Journal of Mathematical Chemistry*, 54(1):252–268, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0559-6`.

Mahalakshmi:2016:ECW

[2583] M. Mahalakshmi and G. Hariharan. An efficient Chebyshev wavelet based analytical algorithm to steady state reaction-diffusion models arising in mathematical chemistry. *Journal of Mathematical Chemistry*, 54(1):269–285, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0560-0.

Fujita:2016:TIEa

[2584] Shinsaku Fujita. Type-itemized enumeration of quadruplets of RS-stereoisomers. I. Cycle indices with chirality fittingness modulated by type-IV quadruplets. *Journal of Mathematical Chemistry*, 54(1):286–309, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0561-z.

Fujita:2016:TIEb

[2585] Shinsaku Fujita. Type-itemized enumeration of quadruplets of RS-stereoisomers: II-cycle indices with chirality fittingness modulated by type-V quadruplets. *Journal of Mathematical Chemistry*, 54(1):310–330, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0562-y.

Alajbegovic:2016:ZFS

[2586] Hermina Alajbegović and Muharem Avdispahić. Zeta functions and subgroup growth in $\mathbf{P2/m}$. *Journal of Mathematical Chemistry*, 54(1):331–343, January 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0563-x.

Cao:2016:TIS

[2587] Shi-Fa Cao, Jun Yin, and Yin-Sheng Huang. Theoretical investigation of the substitution effects on carrier transport properties of tetrathia[22]annulene-[2,1,2,1] derivatives. *Journal of Mathematical Chemistry*, 54(2):345–357, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0583-6.

Koibuchi:2016:STL

[2588] Hiroshi Koibuchi, Andrey Shobukhov, and Hideo Sekino. Surface tension and Laplace pressure in triangulated surface models for membranes without fixed boundary. *Journal of Mathematical Chemistry*, 54(2):358–374, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-015-0564-9.

Alvarez-Ramirez:2016:SRL

[2589] J. Alvarez-Ramirez, R. Femat, M. Meraz, and C. Ibarra-Valdez. Some remarks on the Langmuir–Hinshelwood kinetics. *Journal of Mathematical Chemistry*, 54(2):375–392, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0566-7`.

Strekalov:2016:CTS

[2590] Mikhail L. Strekalov. Classical trajectories as solutions of the Schrödinger equation. *Journal of Mathematical Chemistry*, 54(2):393–402, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0567-6`.

Fu:2016:PLS

[2591] Yingxiong Fu, Jiangtao Peng, and Xuemei Dong. Partial least squares with a regularized weight. *Journal of Mathematical Chemistry*, 54(2):403–415, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0570-y`.

Deng:2016:ECP

[2592] Kecai Deng and Xiaoling Zhang. Enumeration of cyclic polyazulenoids. *Journal of Mathematical Chemistry*, 54(2):416–427, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0569-4`.

Butt:2016:LTK

[2593] Saad Ihsan Butt, Muhammad Numan, and Shahid Qaisar. Labelings of type $(1, 1, 1)$ for Klein bottle fullerenes. *Journal of Mathematical Chemistry*, 54(2):428–441, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0568-5`.

Zhou:2016:NTS

[2594] Zhou Zhou and T. E. Simos. A new two stage symmetric two-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of the radial Schrödinger equation. *Journal of Mathematical Chemistry*, 54(2):442–465, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0571-x`.

Alolyan:2016:FSL

[2595] Ibraheem Alolyan and T. E. Simos. Family of symmetric linear six-step methods with vanished phase-lag and its derivatives and their application to the radial Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 54(2):466–502, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0572-9`.

Campion:2016:ECP

[2596] M. J. Campión, G. Arzamendi, L. M. Gandía, and E. Induráin. Entropy of chemical processes versus numerical representability of orderings. *Journal of Mathematical Chemistry*, 54(2):503–526, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0565-8`.

Das:2016:ABV

[2597] Nilima Das, Randhir Singh, Abdul-Majid Wazwaz, and Jitendra Kumar. An algorithm based on the variational iteration technique for the Bratu-type and the Lane–Emden problems. *Journal of Mathematical Chemistry*, 54(2):527–551, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0575-6`.

Fernandez:2016:ASC

[2598] Francisco M. Fernández. On the algebraic structure of central molecular chirality. *Journal of Mathematical Chemistry*, 54(2):552–558, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0577-4`.

Rosenfeld:2016:FNF

[2599] Vladimir R. Rosenfeld. The fractal nature of folds and the Walsh copolymers. *Journal of Mathematical Chemistry*, 54(2):559–571, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0574-7`.

Lesiuk:2016:CSE

[2600] Michal Lesiuk. Calculation of STOs electron repulsion integrals by ellipsoidal expansion and large-order approximations. *Journal of Mathematical Chemistry*, 54(2):572–591, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0576-5`.

Tikhonov:2016:QAP

[2601] Nikolay A. Tikhonov and Mikhail G. Tokmachev. Qualitative analysis of physical factors that determine activity coefficients of electrolytes. III. Mixtures of electrolytes. *Journal of Mathematical Chemistry*, 54(2): 592–601, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0582-7`.

Belkic:2016:QFP

[2602] Dzevad Belkić and Karen Belkić. Quantification by the fast Padé transform of magnetic resonance spectroscopic data encoded at 1.5 T: implications for brain tumor diagnostics. *Journal of Mathematical Chemistry*, 54 (2):602–655, February 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0578-3`.

Carbo-Dorca:2016:AED

[2603] Ramon Carbó-Dorca. About Erdős discrepancy conjecture. *Journal of Mathematical Chemistry*, 54(3):657–660, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0585-4`.

Tachibana:2016:TDR

[2604] Akitomo Tachibana. Time-dependent renormalization of alpha-oscillators for QED. *Journal of Mathematical Chemistry*, 54(3):661–681, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0587-2`.

Morales:2016:EIC

[2605] Daniel A. Morales. On the evaluation of integrals with Coulomb Sturmian radial functions. *Journal of Mathematical Chemistry*, 54(3): 682–689, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0588-1`.

Wei:2016:PMR

[2606] Shouliu Wei, Xiaoling Ke, and Fenggen Lin. Perfect matchings in random polyomino chain graphs. *Journal of Mathematical Chemistry*, 54 (3):690–697, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0580-9`.

Sizochenko:2016:ISI

[2607] Natalia Sizochenko, Victor Kuz'min, Liudmila Ognichenko, and Jerzy Leszczynski. Introduction of simplex-informational descriptors for QSPR analysis of fullerene derivatives. *Journal of Mathematical Chemistry*, 54 (3):698–706, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0581-8`.

Belkic:2016:FPT

[2608] Dzevad Belkić and Karen Belkić. The fast Padé transform for noisy magnetic resonance spectroscopic data from the prostate: potential contribution to individualized prostate cancer care. *Journal of Mathematical Chemistry*, 54(3):707–764, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0586-3`.

Rosenfeld:2016:PCA

[2609] Vladimir R. Rosenfeld, Andrey A. Dobrynin, Josep M. Oliva, and Juanjo Rué. Pentagonal chains and annuli as models for designing nanostructures from cages. *Journal of Mathematical Chemistry*, 54(3): 765–776, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0584-5`.

Zhang:2016:CES

[2610] Qiumei Zhang and Daqing Jiang. Competitive exclusion in a stochastic chemostat model with Holling type II functional response. *Journal of Mathematical Chemistry*, 54(3):777–791, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-015-0589-0`.

Kyurkchiev:2016:NSG

[2611] Nikolay Kyurkchiev and Svetoslav Markov. On the numerical solution of the general kinetic "K-angle" reaction system. *Journal of Mathematical Chemistry*, 54(3):792–805, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0592-0`.

Arendas:2016:SS

[2612] Péter Árendás, Tibor Furtenbacher, and Attila G. Császár. On spectra of spectra. *Journal of Mathematical Chemistry*, 54(3):806–822, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0591-1`.

Quadras:2016:AEW

[2613] Jasintha Quadras, Krishnan Balasubramanian, and K. Arputha Christy. Analytical expressions for Wiener indices of n-circumscribed peri-condensed benzenoid graphs. *Journal of Mathematical Chemistry*, 54 (3):823–843, March 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0596-9`.

Carbo-Dorca:2016:AIP

[2614] Ramon Carbó-Dorca. About an incoherent precision behavior in LCAO MO theory when a simple diatomic molecule collapses into an atom. *Journal of Mathematical Chemistry*, 54(4):845–848, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0607-x`.

Li:2016:SRC

[2615] Risong Li, Yu Zhao, Ru Jiang, and Hongqing Wang. Some remarks on chaos of a coupled lattice system related with the Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 54(4):849–853, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0616-9`.

Yang:2016:LTB

[2616] Ying Yang and Daqing Jiang. Long-time behavior of a perturbed enzymatic reaction model under negative feedback process by white noise. *Journal of Mathematical Chemistry*, 54(4):854–865, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0590-2`.

Merkli:2016:DCD

[2617] M. Merkli, G. P. Berman, R. T. Sayre, S. Gnanakaran, M. Könenberg, A. I. Nesterov, and H. Song. Dynamics of a chlorophyll dimer in collective and local thermal environments. *Journal of Mathematical Chemistry*, 54 (4):866–917, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0593-z`.

Singh:2016:MHP

[2618] Randhir Singh, Sukhjit Singh, and Abdul-Majid Wazwaz. A modified homotopy perturbation method for singular time dependent Emden–Fowler equations with boundary conditions. *Journal of Mathematical Chemistry*, 54(4):918–931, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0594-y.

Nalewajski:2016:ECD

[2619] Roman F. Nalewajski. On entropy-continuity descriptors of molecular equilibrium states. *Journal of Mathematical Chemistry*, 54(4):932–954, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0595-x; http://link.springer.com/content/pdf/10.1007/s10910-016-0595-x.pdf.

Cinkir:2016:ERK

[2620] Zubeyir Cinkir. Effective resistances and Kirchhoff index of ladder graphs. *Journal of Mathematical Chemistry*, 54(4):955–966, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0597-8.

McGinty:2016:RSD

[2621] Sean McGinty and Giuseppe Pontrelli. On the role of specific drug binding in modelling arterial eluting stents. *Journal of Mathematical Chemistry*, 54(4):967–976, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0618-7; http://link.springer.com/content/pdf/10.1007/s10910-016-0618-7.pdf.

Basic:2016:CPG

[2622] Nino Basić, Patrick W. Fowler, and Tomaz Pisanski. Coronoids, patches and generalised altans. *Journal of Mathematical Chemistry*, 54(4):977–1009, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0599-6.

Alolyan:2016:ISL

[2623] Ibraheem Alolyan and T. E. Simos. An implicit symmetric linear six-step methods with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of the radial Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 54(4):1010–1040, April 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0600-4.

Chan:2016:MMS

[2624] Y. Chan. Modelling and MD simulations on ultra-filtration using graphene sheet. *Journal of Mathematical Chemistry*, 54(5):1041–1056, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0606-y`.

Gong:2016:TPB

[2625] Helin Gong, Xian'an Jin, and Fuji Zhang. Tutte polynomials for benzenoid systems with one branched hexagon. *Journal of Mathematical Chemistry*, 54(5):1057–1071, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0601-3`. See erratum [2664].

Venkatesh:2016:NAS

[2626] S. G. Venkatesh, S. Raja Balachandar, S. K. Ayyaswamy, and K. Balasubramanian. A new approach for solving a model for HIV infection of $\mathbf{CD4}^+$ **T**-cells arising in mathematical chemistry using wavelets. *Journal of Mathematical Chemistry*, 54(5):1072–1082, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0604-0`.

Ruiz:2016:EHC

[2627] María Belén Ruiz. Evaluation of Hylleraas–CI atomic integrals by integration over the coordinates of one electron. IV. An improved algorithm for three-electron kinetic energy integrals. *Journal of Mathematical Chemistry*, 54(5):1083–1109, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0608-9`.

Li:2016:RTE

[2628] Risong Li, Jianjun Wang, Tianxiu Lu, and Ru Jiang. Remark on topological entropy and $\sqrt{\ }$-chaos of a coupled lattice system with non-zero coupling constant related with Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 54(5):1110–1116, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0609-8`.

Flapan:2016:LNW

[2629] Erica Flapan and Kenji Kozai. Linking number and writhe in random linear embeddings of graphs. *Journal of Mathematical Chemistry*, 54 (5):1117–1133, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0610-2.

Strekalov:2016:RFW

[2630] Mikhail L. Strekalov. Revival features in wave packet dynamics of a particle confined in a Morse potential: the binomial distribution. *Journal of Mathematical Chemistry*, 54(5):1134–1145, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0612-0.

Loghambal:2016:MAH

[2631] S. Loghambal and A. J. Agvinos Catherine. Mathematical analysis of the heterogeneous photo-Fenton oxidation of acetic acid on structured catalysts. *Journal of Mathematical Chemistry*, 54(5):1146–1158, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0613-z.

Alolyan:2016:FEE

[2632] Ibraheem Alolyan and T. E. Simos. A family of embedded explicit six-step methods with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation: development and theoretical analysis. *Journal of Mathematical Chemistry*, 54(5):1159–1186, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0611-1.

Liang:2016:NFS

[2633] Minjian Liang and T. E. Simos. A new four stages symmetric two-step method with vanished phase-lag and its first derivative for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 54(5):1187–1211, May 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0615-x.

Carbo-Dorca:2016:DBH

[2634] Ramon Carbó-Dorca. N-dimensional Boolean hypercubes and the Goldbach Conjecture. *Journal of Mathematical Chemistry*, 54(6):1213–1220, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0628-5.

Ivanauskas:2016:ICT

[2635] Feliksas Ivanauskas, Pranas Katauskis, and Valdas Laurinavicius. Impact of convective transport and inert membrane on action of the bio-catalytic

filter. *Journal of Mathematical Chemistry*, 54(6):1221–1232, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0619-6`.

Carrillo:2016:OPC

[2636] Lizeth Carrillo, Jesica A. Escobar, Julio B. Clempner, and Alexander S. Poznyak. Optimization problems in chemical reactions using continuous-time Markov chains. *Journal of Mathematical Chemistry*, 54 (6):1233–1254, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0620-0`.

Roul:2016:NAS

[2637] Pradip Roul and Ujwal Warbhe. New approach for solving a class of singular boundary value problem arising in various physical models. *Journal of Mathematical Chemistry*, 54(6):1255–1285, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0617-8`. See erratum [2638].

Roul:2016:ENA

[2638] Pradip Roul and Ujwal Warbhe. Erratum to: New approach for solving a class of singular boundary value problem arising in various physical models. *Journal of Mathematical Chemistry*, 54(6):1286, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0623-x; http://link.springer.com/content/pdf/10.1007/s10910-016-0623-x.pdf`. See [2637].

Nogueira:2016:LCB

[2639] P. H. F. Nogueira, A. S. de Castro, and D. R. M. Pimentel. A large class of bound-state solutions of the Schrödinger equation via Laplace transform of the confluent hypergeometric equation. *Journal of Mathematical Chemistry*, 54(6):1287–1295, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0621-z`.

Tratnik:2016:DLS

[2640] Niko Tratnik and Petra Zigert Pletersek. Distributive lattice structure on the set of perfect matchings of carbon nanotubes. *Journal of Mathematical Chemistry*, 54(6):1296–1305, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0622-y`.

Skakauskas:2016:NSC

[2641] V. Skakauskas and P. Katauskis. Numerical study of CO oxidation by N_2O reaction over supported catalysts. *Journal of Mathematical Chemistry*, 54(6):1306–1320, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0625-8`.

Fernandez:2016:UTF

[2642] Francisco M. Fernández and Javier Garcia. Unitary transformations of a family of two-dimensional anharmonic oscillators. *Journal of Mathematical Chemistry*, 54(6):1321–1326, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0624-9`.

Drexler:2016:GCC

[2643] Dániel András Drexler and János Tóth. Global controllability of chemical reactions. *Journal of Mathematical Chemistry*, 54(6):1327–1350, June 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0626-7`.

Bayon:2016:SLU

[2644] L. Bayón, J. A. Otero, P. M. Suárez, and C. Tasis. Solving linear unbranched pathways with Michaelis–Menten kinetics using the Lambert W-function. *Journal of Mathematical Chemistry*, 54(7):1351–1369, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-015-0579-2; http://link.springer.com/article/10.1007/s10910-015-0579-2`.

Martinez:2016:LCF

[2645] Eulalia Martínez, Sukhjit Singh, José L. Hueso, and Dharmendra K. Gupta. Local convergence of a family of iterative methods for Hammerstein equations. *Journal of Mathematical Chemistry*, 54(7):1370–1386, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0602-2; http://link.springer.com/article/10.1007/s10910-016-0602-2`.

Bulai:2016:BOP

[2646] Iulia Martina Bulai and Ezio Venturino. Biodegradation of organic pollutants in a water body. *Journal of Mathematical Chemistry*,

54(7):1387–1403, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0603-1; http://link.springer.com/article/10.1007/s10910-016-0603-1.

Argyros:2016:LCC

[2647] Ioannis K. Argyros, Á. Alberto Magreñán, and Lara Orcos. Local convergence and a chemical application of derivative free root finding methods with one parameter based on interpolation. *Journal of Mathematical Chemistry*, 54(7):1404–1416, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0605-z; http://link.springer.com/article/10.1007/s10910-016-0605-z.

Xi:2016:NHA

[2648] Xiaopeng Xi and T. E. Simos. A new high algebraic order four stages symmetric two-step method with vanished phase-lag and its first and second derivatives for the numerical solution of the Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 54(7):1417–1439, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0627-6; http://link.springer.com/article/10.1007/s10910-016-0627-6.

Carbo-Dorca:2016:NCQ

[2649] Ramon Carbó-Dorca. On the nature of the collective quantum mechanical description of molecular atoms and bonds. *Journal of Mathematical Chemistry*, 54(7):1440–1446, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0629-4; http://link.springer.com/article/10.1007/s10910-016-0629-4.

Zachos:2016:WFT

[2650] Anastasios N. Zachos. The weighted Fermat–Torricelli–Menger problem for a given sextuple of edge lengths determining tetrahedra. *Journal of Mathematical Chemistry*, 54(7):1447–1460, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0630-y; http://link.springer.com/article/10.1007/s10910-016-0630-y.

Belkic:2016:IDY

[2651] Dzevad Belkić and Karen Belkić. Improving the diagnostic yield of magnetic resonance spectroscopy for pediatric brain tumors through mathematical optimization. *Journal of Mathematical Chemistry*, 54 (7):1461–1513, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0632-9; http://link.springer.com/article/10.1007/s10910-016-0632-9`.

Leong:2016:AAI

[2652] Chong H. Leong, Ignacio Porras, and Frederick W. King. Analysis of atomic integrals involving explicit correlation factors for the three-electron case. I. Connection to the hypergeometric function ${}_3\vec{F}_2$. *Journal of Mathematical Chemistry*, 54(7):1514–1552, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0633-8; http://link.springer.com/article/10.1007/s10910-016-0633-8`.

Balasubramanian:2016:CPG

[2653] Krishnan Balasubramanian. Combinatorics of Petersen graph and its compositions for all irreducible representations for Jahn–Teller, non-rigid molecules and clusters. *Journal of Mathematical Chemistry*, 54(7):1553–1574, August 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0634-7; http://link.springer.com/article/10.1007/s10910-016-0634-7`.

Andova:2016:DNS

[2654] Vesna Andova, Martin Knor, and Riste Skrekovski. Distances on nanotubical structures. *Journal of Mathematical Chemistry*, 54(8): 1575–1584, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0637-4; http://link.springer.com/article/10.1007/s10910-016-0637-4`.

Zhu:2016:DMF

[2655] Xun Zhu and Yuriko Aoki. Development of molecular fragment interaction method for designing organic ferromagnets. *Journal of Mathematical Chemistry*, 54(8):1585–1595, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0638-3; http://link.springer.com/article/10.1007/s10910-016-0638-3`.

Misra:2016:EAM

[2656] A. K. Misra. Effects of aerosols in making artificial rain: a modeling study. *Journal of Mathematical Chemistry*, 54(8):1596–1611, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0639-2; http://link.springer.com/article/10.1007/s10910-016-0639-2`.

Johnston:2016:LPA

[2657] Matthew D. Johnston. A linear programming approach to dynamical equivalence, linear conjugacy, and the Deficiency One Theorem. *Journal of Mathematical Chemistry*, 54(8):1612–1631, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0640-9; http://link.springer.com/article/10.1007/s10910-016-0640-9`.

Alfifi:2016:NSF

[2658] H. Y. Alfifi, T. R. Marchant, and M. I. Nelson. Non-smooth feedback control for Belousov–Zhabotinskii reaction-diffusion equations: semi-analytical solutions. *Journal of Mathematical Chemistry*, 54 (8):1632–1657, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0641-8; http://link.springer.com/article/10.1007/s10910-016-0641-8`.

Gabor:2016:LCB

[2659] Attila Gábor, Katalin M. Hangos, and Gábor Szederkényi. Linear conjugacy in biochemical reaction networks with rational reaction rates. *Journal of Mathematical Chemistry*, 54(8):1658–1676, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0642-7; http://link.springer.com/article/10.1007/s10910-016-0642-7`.

Rhile:2016:EIP

[2660] Ian J. Rhile. Expressions for the integrated probability density for the hydrogen $2s$ and $2p$ orbitals evaluated within isosurfaces. *Journal of Mathematical Chemistry*, 54(8):1677–1685, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0643-6; http://link.springer.com/article/10.1007/s10910-016-0643-6`.

Onaka:2016:IEL

[2661] Susumu Onaka and Kunio Hayashi. Interpretation of elements of the logarithm of a rotation matrix as rotation components around coordinate axes of a reference frame. *Journal of Mathematical Chemistry*, 54(8):1686–1695, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0644-5; http://link.springer.com/article/10.1007/s10910-016-0644-5`.

Alolyan:2016:NEA

[2662] Ibraheem Alolyan and T. E. Simos. A new eight algebraic order embedded explicit six-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 54(8):1696–1727, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0645-4; http://link.springer.com/article/10.1007/s10910-016-0645-4`.

Arockiaraj:2016:VCM

[2663] Micheal Arockiaraj, S. Ruth Julie Kavitha, and Krishnan Balasubramanian. Vertex cut method for degree and distance-based topological indices and its applications to silicate networks. *Journal of Mathematical Chemistry*, 54(8):1728–1747, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0646-3; http://link.springer.com/article/10.1007/s10910-016-0646-3`.

Gong:2016:ETP

[2664] Helin Gong, Xian'an Jin, and Fuji Zhang. Erratum to: Tutte polynomials for benzenoid systems with one branched hexagon. *Journal of Mathematical Chemistry*, 54(8):1748–1749, September 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0662-3; http://link.springer.com/content/pdf/10.1007/s10910-016-0662-3.pdf`. See [2625].

Carbo-Dorca:2016:TVP

[2665] Ramon Carbó-Dorca. Time vectors and particle swarms defined as polyhedra in spherically enfolded spaces. *Journal of Mathematical Chemistry*, 54(9):1751–1757, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.`

com/accesspage/article/10.1007/s10910-016-0648-1; http://link.springer.com/article/10.1007/s10910-016-0648-1.

Rosenfeld:2016:STS

[2666] Vladimir R. Rosenfeld and Thomas E. Nordahl. Semigroup theory of symmetry. *Journal of Mathematical Chemistry*, 54(9):1758–1776, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0653-4; http://link.springer.com/article/10.1007/s10910-016-0653-4.

Nalewajski:2016:CER

[2667] Roman F. Nalewajski. Complex entropy and resultant information measures. *Journal of Mathematical Chemistry*, 54(9):1777–1782, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0651-6; http://link.springer.com/content/pdf/10.1007/s10910-016-0651-6.pdf.

Nogueira:2016:GMP

[2668] Pedro H. F. Nogueira and Antonio S. de Castro. From the generalized Morse potential to a unified treatment of the D-dimensional singular harmonic oscillator and singular Coulomb potentials. *Journal of Mathematical Chemistry*, 54(9):1783–1791, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0635-6; http://link.springer.com/article/10.1007/s10910-016-0635-6.

Amovilli:2016:AWM

[2669] C. Amovilli and N. H. March. Approaching the s-wave model ground state energy of He-like atomic ions: results from a model Hamiltonian. *Journal of Mathematical Chemistry*, 54(9):1792–1797, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0647-2; http://link.springer.com/article/10.1007/s10910-016-0647-2.

Carbo-Dorca:2016:SGC

[2670] Ramon Carbó-Dorca. A study on Goldbach conjecture. *Journal of Mathematical Chemistry*, 54(9):1798–1809, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0649-0; http://link.springer.com/article/10.1007/s10910-016-0649-0.

Yahya:2016:QIE

[2671] W. A. Yahya, K. J. Oyewumi, and K. D. Sen. Quantum information entropies for the ℓ-state Pöschl–Teller-type potential. *Journal of Mathematical Chemistry*, 54(9):1810–1821, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0650-7; http://link.springer.com/article/10.1007/s10910-016-0650-7.

Bastos:2016:QMP

[2672] Cristiano C. Bastos, Antonio C. Pavão, and Eduardo S. G. Leandro. On the quantum mechanics of a particle constrained to generalized cylinders with application to Möbius strips. *Journal of Mathematical Chemistry*, 54(9):1822–1834, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0652-5; http://link.springer.com/article/10.1007/s10910-016-0652-5.

Alolyan:2016:FTS

[2673] Ibraheem Alolyan and T. E. Simos. A family of two stages tenth algebraic order symmetric six-step methods with vanished phase-lag and its first derivatives for the numerical solution of the radial Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 54(9):1835–1862, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0654-3; http://link.springer.com/article/10.1007/s10910-016-0654-3.

Tobias:2016:FOC

[2674] Roland Tóbiás, László L. Stacho, and Gyula Tasi. First-order chemical reaction networks I: theoretical considerations. *Journal of Mathematical Chemistry*, 54(9):1863–1878, October 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0655-2; http://link.springer.com/article/10.1007/s10910-016-0655-2.

Pota:2016:SDF

[2675] György Póta. Solutions defined on finite time intervals in a model of a real kinetic system. *Journal of Mathematical Chemistry*, 54(10):1879–1883, November 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0664-1; http://link.springer.com/article/10.1007/s10910-016-0664-1.

Plesa:2016:CRS

[2676] Tomislav Plesa, Tomás Vejchodský, and Radek Erban. Chemical reaction systems with a homoclinic bifurcation: an inverse problem. *Journal of Mathematical Chemistry*, 54(10):1884–1915, November 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0656-1; http://link.springer.com/content/pdf/10.1007/s10910-016-0656-1.pdf`.

Prabhu:2016:ISD

[2677] Ganesh Prabhu, Sudeepto Bhattacharya, Michael P. Krein, and N. Sukumar. Investigation of similarity and diversity threshold networks generated from diversity-oriented and focused chemical libraries. *Journal of Mathematical Chemistry*, 54(10):1916–1941, November 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0657-0; http://link.springer.com/article/10.1007/s10910-016-0657-0`.

Kirwan:2016:DE

[2678] A. D. Kirwan, Jr. and William Seitz. Doppelgänger entropies. *Journal of Mathematical Chemistry*, 54(10):1942–1951, November 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0658-z; http://link.springer.com/content/pdf/10.1007/s10910-016-0658-z.pdf`.

Masia:2016:NTP

[2679] Maria D. Masia, Manuela Garcia-Moreno, Francisco Garcia-Sevilla, Julio Escribano, Milagros Molina-Alarcon, Maria L. Amo-Saus, Carmen V. Ortiz-Ruiz, and Ramon Varon. A novel transient phase kinetic analysis of the fractional modification of monocyclic enzyme cascades. *Journal of Mathematical Chemistry*, 54(10):1952–1972, November 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0659-y; http://link.springer.com/article/10.1007/s10910-016-0659-y`.

Marmorino:2016:LBG

[2680] M. G. Marmorino and Voleta Black. Lower bounds to the ground-state expectation value of non-negative operators. *Journal of Mathematical Chemistry*, 54(10):1973–1985, November 2016. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0660-5; http://link.springer.com/article/10.1007/s10910-016-0660-5.

Kuzmin:2016:ETI

[2681] Victor Kuz'min, Lyudmila Ognichenko, Adlen Mouats, Anatoliy Artemenko, Ianina Burdina, Valery Shapkin, Natalia Sizochenko, and Jerzy Leszczynski. Efficacy of topological informational potentials for analysis of nonequivalent atoms in molecular graphs: the case of chiral fullerenes. *Journal of Mathematical Chemistry*, 54(10):1986–1996, November 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0661-4; http://link.springer.com/article/10.1007/s10910-016-0661-4.

Hordijk:2016:ASP

[2682] Wim Hordijk and Mike Steel. Autocatalytic sets in polymer networks with variable catalysis distributions. *Journal of Mathematical Chemistry*, 54(10):1997–2021, November 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0666-z; http://link.springer.com/article/10.1007/s10910-016-0666-z.

Mazur:2016:BFE

[2683] Grzegorz Mazur, Marcin Makowski, and Roman Lazarski. Boys function evaluation on graphical processing units. *Journal of Mathematical Chemistry*, 54(10):2022–2047, November 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0668-x; http://link.springer.com/content/pdf/10.1007/s10910-016-0668-x.pdf.

Fujii:2016:RHF

[2684] Hiroyuki Fujii, Shinpei Okawa, Yukio Yamada, Yoko Hoshi, and Masao Watanabe. Renormalization of the highly forward-peaked phase function using the double exponential formula for radiative transfer. *Journal of Mathematical Chemistry*, 54(10):2048–2061, November 2016. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0670-3; http://link.springer.com/article/10.1007/s10910-016-0670-3.

Zhao:2017:SDA

[2685] Xuezhuang Zhao, Jianxia Cui, Zucheng Li, Xiufang Xu, Zhenfeng Shang, Yun Li, Guichang Wang, and Ruifang Li. Symmetries of deoxyribonucleic acid (DNA) and related molecules. *Journal of Mathematical Chemistry*, 55(1):1–33, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0663-2; http://link.springer.com/article/10.1007/s10910-016-0663-2`.

Kaatz:2017:KMC

[2686] Forrest H. Kaatz, Adhemar Bultheel, and Ottorino Ori. Kinetic Monte Carlo approach to Schottky defects in noble metal nanoclusters. *Journal of Mathematical Chemistry*, 55(1):34–49, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0667-y; http://link.springer.com/article/10.1007/s10910-016-0667-y`.

Thilagam:2017:TMD

[2687] A. Thilagam. Transition-metal dichalcogenide heterostructure solar cells: a numerical study. *Journal of Mathematical Chemistry*, 55(1):50–64, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0669-9; http://link.springer.com/article/10.1007/s10910-016-0669-9`.

Frolov:2017:ACB

[2688] Alexei M. Frolov and David M. Wardlaw. Accurate computations of bound state properties in three- and four-electron atomic systems in the basis of multi-dimensional gaussoids. *Journal of Mathematical Chemistry*, 55(1):65–78, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0671-2; http://link.springer.com/article/10.1007/s10910-016-0671-2`.

Carbo-Dorca:2017:TGM

[2689] Ramon Carbó-Dorca. A theorem on the Gram matrix of a polyhedron. *Journal of Mathematical Chemistry*, 55(1):79–97, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0672-1; http://link.springer.com/article/10.1007/s10910-016-0672-1`.

Ohta:2017:GEE

[2690] Katsuhisa Ohta. Gauging away the electron-electron interaction by the local phase of complex wave functions in two-electron systems. *Journal of Mathematical Chemistry*, 55(1):98–104, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0673-0; http://link.springer.com/article/10.1007/s10910-016-0673-0`.

Alolyan:2017:NTSa

[2691] Ibraheem Alolyan and T. E. Simos. A new two stages tenth algebraic order symmetric six-step method with vanished phase-lag and its first and second derivatives for the solution of the radial Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 55(1):105–131, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0674-z; http://link.springer.com/article/10.1007/s10910-016-0674-z`.

Zhang:2017:EMT

[2692] Xiaoling Zhang and Kecai Deng. Enumeration of Möbius type cyclic polyazulenoids. *Journal of Mathematical Chemistry*, 55(1):132–141, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0675-y; http://link.springer.com/article/10.1007/s10910-016-0675-y`.

Tokmachev:2017:ASS

[2693] Mikhail G. Tokmachev, Nikolai B. Ferapontov, and Alexandr N. Gagarin. Analysis of the swelling or shrinking kinetics of crosslinked hydrophilic polymers by mathematical modeling. *Journal of Mathematical Chemistry*, 55(1):142–152, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0676-x; http://link.springer.com/article/10.1007/s10910-016-0676-x`.

Macias-Diaz:2017:CEM

[2694] Jorge E. Macías-Díaz, Iliana E. Medina-Ramírez, and Axel Chávez-Guzmán. A compact exponential method for the efficient numerical simulation of the dewetting process of viscous thin films. *Journal of Mathematical Chemistry*, 55(1):153–174, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL

http://link.springer.com/accesspage/article/10.1007/s10910-016-0677-9; http://link.springer.com/article/10.1007/s10910-016-0677-9.

Gozukirmizi:2017:PET

[2695] Cosar Gözükirmizi, Melike Ebru Kirkin, and Metin Demiralp. Probabilistic evolution theory for the solution of explicit autonomous ordinary differential equations: squarified telescope matrices. *Journal of Mathematical Chemistry*, 55(1):175–194, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0678-8; http://link.springer.com/article/10.1007/s10910-016-0678-8.

Balasubramanian:2017:NWG

[2696] Krishnan Balasubramanian. Nested wreath groups and their applications to phylogeny in biology and Cayley trees in chemistry and physics. *Journal of Mathematical Chemistry*, 55(1):195–222, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0680-1; http://link.springer.com/article/10.1007/s10910-016-0680-1.

Zhang:2017:EFM

[2697] Yanwei Zhang, Xiong You, and Yonglei Fang. Exponentially fitted multi-derivative linear methods for the resonant state of the Schrödinger equation. *Journal of Mathematical Chemistry*, 55(1):223–237, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0683-y; http://link.springer.com/article/10.1007/s10910-016-0683-y.

Zhang:2017:NPF

[2698] Ruqiang Zhang, Wenjuan Jiang, Julius Osato Ehigie, Yonglei Fang, and Xiong You. Novel phase-fitted symmetric splitting methods for chemical oscillators. *Journal of Mathematical Chemistry*, 55(1):238–258, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0684-x; http://link.springer.com/article/10.1007/s10910-016-0684-x.

Yang:2017:RKN

[2699] Yanping Yang, Xiong You, and Yonglei Fang. Runge–Kutta–Nyström methods with equation dependent coefficients and reduced phase

lag for oscillatory problems. *Journal of Mathematical Chemistry*, 55(1):259–277, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0685-9; http://link.springer.com/article/10.1007/s10910-016-0685-9`.

Li:2017:HDM

[2700] Genyuan Li, Xi Xing, William Welsh, and Herschel Rabitz. High dimensional model representation constructed by support vector regression. I. Independent variables with known probability distributions. *Journal of Mathematical Chemistry*, 55(1):278–303, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0690-z; http://link.springer.com/article/10.1007/s10910-016-0690-z`.

Belkic:2017:IAS

[2701] Dzevad Belkić and Karen Belkić. Iterative averaging of spectra as a powerful way of suppressing spurious resonances in signal processing. *Journal of Mathematical Chemistry*, 55(1):304–348, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0693-9; http://link.springer.com/content/pdf/10.1007/s10910-016-0693-9.pdf`.

Belkic:2017:VMR

[2702] Dzevad Belkić and Karen Belkić. In vivo magnetic resonance spectroscopy for ovarian cancer diagnostics: quantification by the fast Padé transform. *Journal of Mathematical Chemistry*, 55(1):349–405, January 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/article/10.1007/s10910-016-0694-8; http://link.springer.com/content/pdf/10.1007/s10910-016-0694-8.pdf`.

Strekalov:2017:PRT

[2703] Mikhail L. Strekalov. The perfect revival time of localized wave packet consisting of superposition of bound states with an arbitrary energy spectrum. *Journal of Mathematical Chemistry*, 55(2):407–412, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0700-1; http://link.springer.com/article/10.1007/s10910-016-0700-1`.

Shizgal:2017:CRI

[2704] Bernie D. Shizgal, Nicholas Ho, and Xingwei Yang. The computation of radial integrals with nonclassical quadratures for quantum chemistry and other applications. *Journal of Mathematical Chemistry*, 55(2):413–422, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0689-5; http://link.springer.com/article/10.1007/s10910-016-0689-5`.

Alexander:2017:PRR

[2705] William A. Alexander. Performance of a rigid rod statistical mechanical treatment to predict monolayer ordering: a study of chain interactions and comparison with molecular dynamics simulation. *Journal of Mathematical Chemistry*, 55(2):423–435, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0682-z; http://link.springer.com/article/10.1007/s10910-016-0682-z`.

Turulski:2017:DGF

[2706] Jan Turulski. Dimension of the Gibbs function topological manifold: 3. Configuration entropy determined by the isotopic composition of binary quasicrystals. *Journal of Mathematical Chemistry*, 55(2):436–454, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0686-8; http://link.springer.com/article/10.1007/s10910-016-0686-8`.

Ozay:2017:WTM

[2707] Evrim Korkmaz Özay and Metin Demiralp. Weighted tridiagonal matrix enhanced multivariance products representation (WTMEMPR) for decomposition of multiway arrays: applications on certain chemical system data sets. *Journal of Mathematical Chemistry*, 55(2):455–476, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-016-0687-7; http://link.springer.com/article/10.1007/s10910-016-0687-7`.

Paldus:2017:EIC

[2708] Josef Paldus. Externally and internally corrected coupled cluster approaches: an overview. *Journal of Mathematical Chemistry*, 55(2):477–502, February 2017. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0688-6; http://link.springer.com/article/10.1007/s10910-016-0688-6.

Alolyan:2017:NTSb

[2709] Ibraheem Alolyan and T. E. Simos. New two stages high order symmetric six-step method with vanished phase-lag and its first, second and third derivatives for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 55(2):503–531, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0691-y; http://link.springer.com/article/10.1007/s10910-016-0691-y.

Houjou:2017:MII

[2710] Hirohiko Houjou. Modelling intra- and intermolecular vibrations under the harmonic oscillator approximation: from symmetry-adapted to coarse-grained coordinate approaches. *Journal of Mathematical Chemistry*, 55(2):532–551, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0692-x; http://link.springer.com/article/10.1007/s10910-016-0692-x.

Milani:2017:CFN

[2711] G. Milani and F. Milani. Closed form numerical approach for a kinetic interpretation of high-cis polybutadiene rubber vulcanization with sulphur. *Journal of Mathematical Chemistry*, 55(2):552–583, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0695-7; http://link.springer.com/article/10.1007/s10910-016-0695-7.

Avery:2017:CRC

[2712] James Emil Avery and John Scales Avery. A chainlike relative coordinate system for few-particle problems. *Journal of Mathematical Chemistry*, 55(2):584–597, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0696-6; http://link.springer.com/article/10.1007/s10910-016-0696-6.

Molski:2017:ESC

[2713] Marcin Molski. Exact solutions and coherent states for a generalized potential. *Journal of Mathematical Chemistry*, 55(2):598–606, February

2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/article/10.1007/s10910-016-0697-5; http://link.springer.com/content/pdf/10.1007/s10910-016-0697-5.pdf.

Gluzman:2017:ASS

[2714] S. Gluzman and V. I. Yukalov. Additive self-similar approximants. *Journal of Mathematical Chemistry*, 55(2):607–622, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0698-4; http://link.springer.com/article/10.1007/s10910-016-0698-4.

Fernandez:2017:TDK

[2715] Francisco M. Fernández and Javier Garcia. On two different kinds of resonances in one-dimensional quantum-mechanical models. *Journal of Mathematical Chemistry*, 55(2):623–631, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0699-3; http://link.springer.com/article/10.1007/s10910-016-0699-3.

Luo:2017:FCH

[2716] Xiaopeng Luo, Xin Xu, and Herschel Rabitz. On the fundamental conjecture of HDMR: a Fourier analysis approach. *Journal of Mathematical Chemistry*, 55(2):632–660, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0701-0; http://link.springer.com/article/10.1007/s10910-016-0701-0.

Mamedov:2017:AEZ

[2717] B. A. Mamedov and E. Somuncu. Analytical evaluation of zero-pressure Joule–Thomson coefficient using second virial coefficient and its application. *Journal of Mathematical Chemistry*, 55(2):661–672, February 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0702-z; http://link.springer.com/article/10.1007/s10910-016-0702-z.

Mittal:2017:SOD

[2718] R. C. Mittal and Rajni Rohila. A study of one dimensional nonlinear diffusion equations by Bernstein polynomial based differential quadrature method. *Journal of Mathematical Chemistry*, 55(2):673–695, February

2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0703-y; http://link.springer.com/article/10.1007/s10910-016-0703-y.

Zhao:2017:NFA

[2719] Jianbin Zhao and T. E. Simos. A new fourteenth algebraic order finite difference method for the approximate solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 55(3):697–716, March 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0704-x; http://link.springer.com/article/10.1007/s10910-016-0704-x.

Wang:2017:EEO

[2720] Zhiwei Wang and T. E. Simos. An economical eighth-order method for the approximation of the solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 55(3):717–733, March 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0718-4; http://link.springer.com/article/10.1007/s10910-016-0718-4.

Mamode:2017:CMC

[2721] Malik Mamode. Computation of the Madelung constant for hypercubic crystal structures in any dimension. *Journal of Mathematical Chemistry*, 55(3):734–751, March 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0705-9; http://link.springer.com/article/10.1007/s10910-016-0705-9.

Deza:2017:LLS

[2722] Michel-Marie Deza and Mathieu Dutour Sikirić. Lego-like spheres and tori. *Journal of Mathematical Chemistry*, 55(3):752–798, March 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0706-8; http://link.springer.com/article/10.1007/s10910-016-0706-8.

Wazwaz:2017:VIM

[2723] Abdul-Majid Wazwaz. The variational iteration method for solving systems of third-order Emden–Fowler type equations. *Journal of Mathematical Chemistry*, 55(3):799–817, March 2017. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0707-7; http://link.springer.com/article/10.1007/s10910-016-0707-7.

Das:2017:TPF

[2724] Debojyoti Das. Turing pattern formation in anisotropic medium. *Journal of Mathematical Chemistry*, 55(3):818–831, March 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0709-5; http://link.springer.com/article/10.1007/s10910-016-0709-5.

Lente:2017:ASR

[2725] Gábor Lente. Analytical solutions for the rate equations of irreversible two-step consecutive processes with mixed second order later steps. *Journal of Mathematical Chemistry*, 55(3):832–848, March 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0712-x; http://link.springer.com/article/10.1007/s10910-016-0712-x.

Imran:2017:SFA

[2726] Shahid Imran, Muhammad Hussain, Muhammad Kamran Siddiqui, and Muhammad Numan. Super face d-antimagic labeling for disjoint union of toroidal fullerenes. *Journal of Mathematical Chemistry*, 55(3):849–863, March 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0713-9; http://link.springer.com/article/10.1007/s10910-016-0713-9.

Jang:2017:QPM

[2727] Eun Ji Jang, Young Kyu Lee, and Won Sang Chung. A quantum particle in a moving finite harmonic potential. *Journal of Mathematical Chemistry*, 55(3):864–872, March 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0715-7; http://link.springer.com/article/10.1007/s10910-016-0715-7.

Fan:2017:BBO

[2728] Yuan-Jia Fan and Bih-Yaw Jin. From the "Brazuca" ball to octahedral fullerenes: their construction and classification. *Journal of Mathematical Chemistry*, 55(3):873–886, March 2017. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0719-3; http://link.springer.com/article/10.1007/s10910-016-0719-3.

Saha:2017:ILC

[2729] Sandip Saha and Gautam Gangopadhyay. Isochronicity and limit cycle oscillation in chemical systems. *Journal of Mathematical Chemistry*, 55(3):887–910, March 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0729-1; http://link.springer.com/article/10.1007/s10910-016-0729-1.

Nadarajah:2017:MPH

[2730] S. Nadarajah and J. Chu. On moments of powers of the Hulthén density. *Journal of Mathematical Chemistry*, 55(4):911–913, April 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0717-5; http://link.springer.com/article/10.1007/s10910-016-0717-5.

Carbo-Dorca:2017:NVS

[2731] Ramon Carbó-Dorca. Natural vector spaces (inward power and Minkowski norm of a Natural Vector, Natural Boolean Hypercubes) and a Fermat's Last Theorem conjecture. *Journal of Mathematical Chemistry*, 55(4):914–940, April 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0708-6; http://link.springer.com/article/10.1007/s10910-016-0708-6.

Basilevsky:2017:CTK

[2732] Mikhail V. Basilevsky and Ekaterina A. Bormotova. Charge transfer kinetics in non-polar media including a local molecular mode: the temperature dependence in wide ranges. *Journal of Mathematical Chemistry*, 55(4):941–960, April 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0710-z; http://link.springer.com/article/10.1007/s10910-016-0710-z.

Medvedev:2017:TSS

[2733] Maxim A. Medvedev and T. E. Simos. Two stages six-step method with eliminated phase-lag and its first, second, third and fourth derivatives for the approximation of the Schrödinger equation. *Journal of Mathematical Chemistry*, 55(4):961–986, April 2017. CODEN JMCHEG. ISSN

0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0711-y; http://link.springer.com/article/10.1007/s10910-016-0711-y.

Berg:2017:HOC

[2734] Dmitriy B. Berg and T. E. Simos. High order computationally economical six-step method with vanished phase-lag and its derivatives for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 55(4):987–1013, April 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0714-8; http://link.springer.com/article/10.1007/s10910-016-0714-8.

Diudea:2017:TCG

[2735] Mircea V. Diudea and Vladimir R. Rosenfeld. The truncation of a cage graph. *Journal of Mathematical Chemistry*, 55(4):1014–1020, April 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0716-6; http://link.springer.com/article/10.1007/s10910-016-0716-6.

Estrada:2017:AM

[2736] Ernesto Estrada. The ABC matrix. *Journal of Mathematical Chemistry*, 55(4):1021–1033, April 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0725-5; http://link.springer.com/article/10.1007/s10910-016-0725-5.

Xu:2017:TDS

[2737] Chuang Xu. Threshold dynamics of a stochastic Keizer's model with stochastic incidence. *Journal of Mathematical Chemistry*, 55(4):1034–1045, April 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-016-0730-8; http://link.springer.com/article/10.1007/s10910-016-0730-8.

Killingbeck:2017:ANJ

[2738] J. P. Killingbeck and A. Lakhlifi. Accurate numerical JWKB calculations for the quartic oscillator. *Journal of Mathematical Chemistry*, 55(4):1046–1052, April 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL http://link.springer.com/accesspage/article/10.1007/s10910-017-0734-z; http://link.springer.com/article/10.1007/s10910-017-0734-z.

Cao:2017:OCM

[2739] Dewen Cao, Yaoxiong Wang, Shouzhi Li, Ling Yang, Feng Shuang, and Fang Gao. Optimal control of multiple two-photon transitions. *Journal of Mathematical Chemistry*, 55(4):1053–1066, April 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `http://link.springer.com/accesspage/article/10.1007/s10910-017-0735-y; http://link.springer.com/article/10.1007/s10910-017-0735-y`.

Belkic:2017:SSA

[2740] Dzevad Belkić and Karen Belkić. Synergism of spectra averaging and extrapolation for quantification of in vivo MRS time signals encoded from the ovary. *Journal of Mathematical Chemistry*, 55(5):1067–1109, May 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/content/pdf/10.1007/s10910-016-0728-2.pdf`.

Belkic:2017:EVT

[2741] Dzevad Belkić and Karen Belkić. Encoded in vivo time signals from the ovary in magnetic resonance spectroscopy: poles and zeros as the cornerstone for stability of response functions of systems to external perturbations. *Journal of Mathematical Chemistry*, 55(5):1110–1157, May 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/content/pdf/10.1007/s10910-017-0743-y.pdf`.

Gomes:2017:CLS

[2742] F. M. Gomes, J. M. Martínez, and M. Raydan. On the computation of large-scale self-consistent-field iterations. *Journal of Mathematical Chemistry*, 55(5):1158–1172, May 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Zhao:2017:QCT

[2743] Ningjiu Zhao and Yufang Liu. Quasi-classical trajectory insight into stereodynamics for reaction He + $D_2^+ \rightarrow HeD^+ + D$ with the improved potential energy surface. *Journal of Mathematical Chemistry*, 55(5):1173–1186, May 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Huang:2017:PCW

[2744] Z. Huang, H. S. Sidhu, I. N. Towers, Z. Jovanoski, and V. V. Gubernov. Properties of combustion waves in a model with competitive exothermic

reactions. *Journal of Mathematical Chemistry*, 55(5):1187–1201, May 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Yardimci:2017:SDS

[2745] Seyhmus Yardimci, Esra Kir Arpat, and Çagla Can. On the structure of discrete spectrum of a non-selfadjoint system of differential equations with integral boundary condition. *Journal of Mathematical Chemistry*, 55(5):1202–1212, May 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Berg:2017:TSS

[2746] Dmitriy B. Berg and T. E. Simos. Three stages symmetric six-step method with eliminated phase-lag and its derivatives for the solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 55 (5):1213–1235, May 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Basilevsky:2017:MRT

[2747] M. V. Basilevsky and A. I. Voronin. The mass renormalization for the translational Brownian motion. *Journal of Mathematical Chemistry*, 55 (5):1236–1252, May 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Demiralp:2017:ZIL

[2748] Metin Demiralp and Süha Tuna. Zero interval limit perturbation expansion for the spectral entities of Hilbert–Schmidt operators combined with most dominant spectral component extraction: formulation and certain technicalities. *Journal of Mathematical Chemistry*, 55(6):1253–1277, June 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Tuna:2017:ZIL

[2749] Süha Tuna and Metin Demiralp. Zero interval limit perturbation expansion for the spectral entities of Hilbert–Schmidt operators combined with most dominant spectral component extraction: convergence and confirmative implementations. *Journal of Mathematical Chemistry*, 55 (6):1278–1300, June 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Lu:2017:CWM

[2750] Nan Lu, Yuxiang Bu, and Guimei Luo. Cu-wire-mediated dipyrimidine base pairs as the building blocks for conductive and magnetic Cu–DNA

nanowires. *Journal of Mathematical Chemistry*, 55(6):1301–1321, June 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Chen:2017:KEP

[2751] Yu-Hsin Chen and Sheng D. Chao. The kinetic energy partition method applied to quantum eigenvalue problems with many harmonic-oscillator potentials. *Journal of Mathematical Chemistry*, 55(6):1322–1341, June 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). See comment [2872].

Minuzzi:2017:DRM

[2752] F. C. Minuzzi, C. Bublitz, and A. L. De Bortoli. Development of a reduced mechanism for ethanol using directed relation graph and sensitivity analysis. *Journal of Mathematical Chemistry*, 55(6):1342–1359, June 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Sakiyama:2017:ECO

[2753] Hiroshi Sakiyama and Katsushi Waki. Enumeration of conformers for octahedral $[MX(AB)_5]$ and $[MX(ABC)_5]$ complexes on the basis of computational group theory. *Journal of Mathematical Chemistry*, 55(6):1360–1366, June 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Vigo-Aguiar:2017:RMC

[2754] Jesús Vigo-Aguiar and Higinio Ramos. Recent mathematical–computational techniques and models in chemistry. *Journal of Mathematical Chemistry*, 55(7):1367–1369, August 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/content/pdf/10.1007/s10910-017-0758-4.pdf`.

Calvo:2017:CPO

[2755] Florent Calvo and Ersin Yurtsever. Coating of C_{60} by para-H_2 and ortho-D_2: revisiting the solvation shell. *Journal of Mathematical Chemistry*, 55(7):1370–1375, August 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Hernandez:2017:GAI

[2756] Juan C. Hernández, José M. Rodríguez, and José M. Sigarreta. On the geometric–arithmetic index by decompositions. *Journal of Mathematical Chemistry*, 55(7):1376–1391, August 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Argyros:2017:CNM

[2757] I. K. Argyros, J. A. Ezquerro, M. A. Hernández-Verón, and Á. A. Magreñán. Convergence of Newton's method under Vertgeim conditions: new extensions using restricted convergence domains. *Journal of Mathematical Chemistry*, 55(7):1392–1406, August 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Senel:2017:DSB

[2758] P. Senel and M. Tezer-Sezgin. DRBEM solution of biomagnetic fluid flow and heat transfer in cavities. *Journal of Mathematical Chemistry*, 55(7): 1407–1426, August 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Argyros:2017:LCR

[2759] I. K. Argyros, Á. A. Magreñán, L. Orcos, and J. A. Sicilia. Local convergence of a relaxed two-step Newton like method with applications. *Journal of Mathematical Chemistry*, 55(7):1427–1442, August 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Cordero:2017:FPS

[2760] Alicia Cordero, Juan R. Torregrosa, and María P. Vassileva. A family of parametric schemes of arbitrary even order for solving nonlinear models. *Journal of Mathematical Chemistry*, 55(7):1443–1460, August 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Cordero:2017:MSA

[2761] Alicia Cordero, Javier G. Maimó, Juan R. Torregrosa, and María P. Vassileva. Multidimensional stability analysis of a family of biparametric iterative methods. *Journal of Mathematical Chemistry*, 55(7):1461–1480, August 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Bulai:2017:TMM

[2762] Iulia Martina Bulai and Ezio Venturino. Two mathematical models for dissolved oxygen in a lake. *Journal of Mathematical Chemistry*, 55(7): 1481–1504, August 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Magrenan:2017:NIC

[2763] Á. Alberto Magreñán, Ioannis K. Argyros, and Juan Antonio Sicilia. New improved convergence analysis for Newton-like methods with applications. *Journal of Mathematical Chemistry*, 55(7):1505–1520, August

2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Berg:2017:ESS

[2764] Dmitriy B. Berg and T. E. Simos. An efficient six-step method for the solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 55(8):1521–1547, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Dillon:2017:OIP

[2765] Joseph Dillon. On the origins of intersecting potential energy surfaces. *Journal of Mathematical Chemistry*, 55(8):1548–1588, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Restrepo:2017:JMC

[2766] Guillermo Restrepo and Peter Willett. The *Journal of Mathematical Chemistry*: a bibliometric profile. *Journal of Mathematical Chemistry*, 55(8):1589–1596, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Ke:2017:RQP

[2767] Min Ke, Shan Wu, and Chuanhou Gao. Realizations of quasi-polynomial systems and application for stability analysis. *Journal of Mathematical Chemistry*, 55(8):1597–1621, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Tratnik:2017:GPI

[2768] Niko Tratnik. The Graovac–Pisanski index of zig-zag tubulenes and the generalized cut method. *Journal of Mathematical Chemistry*, 55(8):1622–1637, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Thylwe:2017:NFS

[2769] Karl-Erik Thylwe and Patrick McCabe. Near/far-side angular decompositions of Legendre polynomials using the amplitude–phase method. *Journal of Mathematical Chemistry*, 55(8):1638–1648, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/content/pdf/10.1007/s10910-017-0752-x.pdf`.

Ma:2017:ECE

[2770] Jing Ma and T. E. Simos. An efficient and computational effective method for second order problems. *Journal of Mathematical Chemistry*,

55(8):1649–1668, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Basic:2017:SPC

[2771] Nino Basić, Gunnar Brinkmann, Patrick W. Fowler, Tomaz Pisanski, and Nico Van Cleemput. Sizes of pentagonal clusters in fullerenes. *Journal of Mathematical Chemistry*, 55(8):1669–1682, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Belov:2017:AHC

[2772] G. V. Belov, N. M. Aristova, I. V. Morozov, and M. A. Sineva. On approximation of the heat capacity of substances in the gaseous state. *Journal of Mathematical Chemistry*, 55(8):1683–1697, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Belkic:2017:VHC

[2773] Dzevad Belkić and Karen Belkić. Visualizing hidden components of envelopes non-parametrically in magnetic resonance spectroscopy: Phosphocholine, a breast cancer biomarker. *Journal of Mathematical Chemistry*, 55(8):1698–1723, September 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/content/pdf/10.1007/s10910-017-0769-1.pdf`.

Wu:2017:AAS

[2774] Xiaoxuan Wu and Tasso J. Kaper. Analysis of the approximate slow invariant manifold method for reactive flow equations. *Journal of Mathematical Chemistry*, 55(9):1725–1754, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Yang:2017:EEH

[2775] Lan Yang and T. E. Simos. An efficient and economical high order method for the numerical approximation of the Schrödinger equation. *Journal of Mathematical Chemistry*, 55(9):1755–1778, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Nurislamova:2017:MRC

[2776] Liana Fanurovna Nurislamova and Irek Marsovich Gubaydullin. Mechanism reduction of chemical reaction based on sensitivity analysis: development and testing of some new procedure. *Journal of Mathematical Chemistry*, 55(9):1779–1792, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Bieniasz:2017:SCR

[2777] Lesław K. Bieniasz. A specialised cyclic reduction algorithm for linear algebraic equation systems with quasi-tridiagonal matrices. *Journal of Mathematical Chemistry*, 55(9):1793–1807, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/content/pdf/10.1007/s10910-017-0761-9.pdf`.

Konguetsof:2017:GFT

[2778] A. Konguetsof. A generator of families of two-step numerical methods with free parameters and minimal phase-lag. *Journal of Mathematical Chemistry*, 55(9):1808–1832, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Selmi:2017:HFH

[2779] Saranah Selmi, Dan J. Mitchell, Valipuram S. Manoranjan, and Nikolaos K. Voulgarakis. A hybrid fluctuating hydrodynamics and kinetic Monte Carlo method for modeling chemically-powered nanoscale motion. *Journal of Mathematical Chemistry*, 55(9):1833–1848, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Sahin:2017:EET

[2780] E. Sahin, T. Ozdogan, and M. Orbay. On the effectiveness of exponential type orbitals with hyperbolic cosine functions in atomic calculations. *Journal of Mathematical Chemistry*, 55(9):1849–1856, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). See correction [2810].

Pasca:2017:TIT

[2781] Roxana-Diana Pasca, Atena Moldovan, Ossi Horovitz, and Alexandru Lupan. Thermodynamic investigation of tautomerism in triazine oximes. *Journal of Mathematical Chemistry*, 55(9):1857–1868, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Carbo-Dorca:2017:RGF

[2782] Ramon Carbó-Dorca, Camelia Muñoz-Caro, Alfonso Niño, and Sebastián Reyes. Refinement of a generalized Fermat's last theorem conjecture in natural vector spaces. *Journal of Mathematical Chemistry*, 55(9):1869–1877, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Xiao:2017:PMR

[2783] Chuanqi Xiao, Haiyan Chen, and Lu Liu. Perfect matchings in random pentagonal chains. *Journal of Mathematical Chemistry*, 55(9):1878–1886, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic).

Barthel:2017:ETE

[2784] Senja Barthel and Dorothy Buck. Erratum to: Toroidal embeddings of abstractly planar graphs are knotted or linked. *Journal of Mathematical Chemistry*, 55(9):1887, October 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/content/pdf/10.1007/s10910-017-0780-6.pdf`. See [2542].

Cedillo:2017:CLD

[2785] Andrés Cedillo. Comment on "Localization-delocalization phenomena in a cyclic box" by H. H. Corzo, H. G. Laguna, and R. P. Sagar. *Journal of Mathematical Chemistry*, 55(10):1889–1892, November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0776-2`. See [1917].

Kwiatkowski:2017:AMS

[2786] Mirosław Kwiatkowski. Analysis of the microporous structure of the low-cost activated carbon fibres obtained from flax and jute cloth. *Journal of Mathematical Chemistry*, 55(10):1893–1902, November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0768-2`.

Tang:2017:MDE

[2787] Aihua Tang, Guangzhong Hu, and Ming Liu. Mechanical degradation of electrode materials within single particle model in Li-ion batteries for electric vehicles. *Journal of Mathematical Chemistry*, 55(10):1903–1915, November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0770-8`.

Mirdha:2017:CBP

[2788] Rijaul Haque Mirdha and Pinaki Chaudhury. Constructing a bunch of paths for conformational changes in size specific noble gas cluster: a study using a stochastic procedure. *Journal of Mathematical Chemistry*, 55(10):1916–1933, November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0771-7`.

Gutman:2017:EMF

[2789] Ivan Gutman, Slavko Radenković, Sladana Đordević, Igor Z. Milovanović, and Emina I. Milovanović. Extending the McClelland formula for total π-electron energy. *Journal of Mathematical Chemistry*, 55(10): 1934–1940, November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0772-6`.

Rosenfeld:2017:TUC

[2790] Vladimir R. Rosenfeld. The toroidal unit cell of a quasicrystal. *Journal of Mathematical Chemistry*, 55(10):1941–1950, November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0773-5`.

Pratama:2017:ADM

[2791] Satrya Fajri Pratama, Azah Kamilah Muda, Yun-Huoy Choo, Jan Flusser, and Ajith Abraham. ATS drugs molecular structure representation using refined 3D geometric moment invariants. *Journal of Mathematical Chemistry*, 55(10):1951–1963, November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0775-3`.

Zuniga:2017:QSC

[2792] José Zúñiga, Adolfo Bastida, and Alberto Requena. Quantum solution of coupled harmonic oscillator systems beyond normal coordinates. *Journal of Mathematical Chemistry*, 55(10):1964–1984, November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0777-1`.

FerreiraFlorindo:2017:MCT

[2793] Caio César Ferreira Florindo, Christina Papenfuss, and Adalberto Bono Maurizio Sacchi Bassi. Mesoscopic continuum thermodynamics for mixtures of particles with orientation. *Journal of Mathematical Chemistry*, 55(10):1985–2003, November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0778-0`.

Belkic:2017:RIC

[2794] Dzevad Belkić and Karen Belkić. Robust identification of the cancer biomarker phosphocholine through partitioned envelopes in noisy magnetic resonance spectroscopic data by the non-parametric fast Padé transform. *Journal of Mathematical Chemistry*, 55(10):2004–2047,

November 2017. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0807-z; https://link.springer.com/content/pdf/10.1007/s10910-017-0807-z.pdf.

Medvedev:2018:MMO

[2795] Maxim A. Medvedev and T. E. Simos. A multistep method with optimal properties for second order differential equations. *Journal of Mathematical Chemistry*, 56(1):1–29, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0774-4.

Mohamed:2018:CRD

[2796] Fatma Mohamed, Casian Pantea, and Adrian Tudorascu. Chemical reaction-diffusion networks: convergence of the method of lines. *Journal of Mathematical Chemistry*, 56(1):30–68, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0779-z.

Klavzar:2018:PDG

[2797] Sandi Klavzar and M. J. Nadjafi-Arani. Partition distance in graphs. *Journal of Mathematical Chemistry*, 56(1):69–80, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0781-5.

Kovalnogov:2018:FSN

[2798] Vladislav N. Kovalnogov, Ruslan V. Fedorov, Viktor M. Golovanov, Boris M. Kostishko, and T. E. Simos. A four stages numerical pair with optimal phase and stability properties. *Journal of Mathematical Chemistry*, 56(1):81–102, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0782-4.

Thackston:2018:EAD

[2799] Russell Thackston and Ryan C. Fortenberry. An efficient algorithm for the determination of force constants and displacements in numerical definitions of a large, general order Taylor series expansion. *Journal of Mathematical Chemistry*, 56(1):103–119, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0783-3.

Campo:2018:NAD

[2800] Marco Campo, José R. Fernández, María del Carmen Muñiz, and Cristina Núñez. Numerical analysis of a dynamic problem involving bulk-surface surfactants. *Journal of Mathematical Chemistry*, 56(1): 120–139, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0784-2`.

Kryven:2018:ARP

[2801] Ivan Kryven. Analytic results on the polymerisation random graph model. *Journal of Mathematical Chemistry*, 56(1):140–157, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0785-1; https://link.springer.com/content/pdf/10.1007/s10910-017-0785-1.pdf`.

Chan:2018:ASN

[2802] Yue Chan, Bisheng Wu, Yong Ren, and Liang Xia. Analytical solution for Newtonian flow inside carbon nanotube taking into consideration van der Waals forces. *Journal of Mathematical Chemistry*, 56(1): 158–169, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0786-0`.

Yan:2018:FDP

[2803] Ke Yan and T. E. Simos. A finite difference pair with improved phase and stability properties. *Journal of Mathematical Chemistry*, 56(1): 170–192, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0787-z`.

Alon:2018:IAS

[2804] Gil Alon and Inbal Tuvi-Arad. Improved algorithms for symmetry analysis: structure preserving permutations. *Journal of Mathematical Chemistry*, 56(1):193–212, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0788-y`.

Wirth:2018:DMS

[2805] Karl Wirth. Determining the metric and the symmetry group of finite point sets in space with an application to cyclohexane. *Journal of Mathematical Chemistry*, 56(1):213–231, January 2018. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0789-x.

Singh:2018:ENL

[2806] Randheer Singh and J. Jena. On evolution of non-linear waves in polytropic reacting gases. *Journal of Mathematical Chemistry*, 56(1): 232–246, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0790-4.

Jia:2018:NAD

[2807] Ji-Teng Jia. Numerical algorithms for the determinant evaluation of general Hessenberg matrices. *Journal of Mathematical Chemistry*, 56(1): 247–256, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0794-0.

Li:2018:SFO

[2808] Yuanlu Li and Min Jiang. Spatial-fractional order diffusion filtering. *Journal of Mathematical Chemistry*, 56(1):257–267, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0795-z.

Belkic:2018:EQN

[2809] Dzevad Belkić and Karen Belkić. Exact quantification by the non-parametric fast Padé transform using only shape estimation of high-order derivatives of envelopes. *Journal of Mathematical Chemistry*, 56(1):268–314, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0837-6; https://link.springer.com/content/pdf/10.1007/s10910-017-0837-6.pdf.

Sahin:2018:CEE

[2810] E. Sahin, T. Ozdogan, and M. Orbay. Correction to: On the effectiveness of exponential type orbitals with hyperbolic cosine functions in atomic calculations. *Journal of Mathematical Chemistry*, 56(1):315, January 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0820-2; https://link.springer.com/content/pdf/10.1007/s10910-017-0820-2.pdf. See [2780].

Liemert:2018:FRT

[2811] André Liemert and Alwin Kienle. Fractional radiative transport in the diffusion approximation. *Journal of Mathematical Chemistry*, 56(2): 317–335, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0792-2`.

Cortez:2018:CAL

[2812] Mark Jayson Cortez, Allen Nazareno, and Eduardo Mendoza. A computational approach to linear conjugacy in a class of power law kinetic systems. *Journal of Mathematical Chemistry*, 56(2):336–357, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0796-y; https://link.springer.com/content/pdf/10.1007/s10910-017-0796-y.pdf`.

Talabis:2018:PEC

[2813] Dylan Antonio S. J. Talabis, Carlene Perpetua P. Arceo, and Eduardo R. Mendoza. Positive equilibria of a class of power-law kinetics. *Journal of Mathematical Chemistry*, 56(2):358–394, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0804-2; https://link.springer.com/content/pdf/10.1007/s10910-017-0804-2.pdf`.

Arceo:2018:RSK

[2814] Carlene Perpetua P. Arceo, Editha C. Jose, Angelyn R. Lao, and Eduardo R. Mendoza. Reactant subspaces and kinetics of chemical reaction networks. *Journal of Mathematical Chemistry*, 56(2):395–422, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0809-x; https://link.springer.com/content/pdf/10.1007/s10910-017-0809-x.pdf`.

Fang:2018:HFD

[2815] Jie Fang, Chenglian Liu, and T. E. Simos. A hybrid finite difference pair with maximum phase and stability properties. *Journal of Mathematical Chemistry*, 56(2):423–448, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0793-1`.

Yao:2018:NFD

[2816] Junfeng Yao and T. E. Simos. New finite difference pair with optimized phase and stability properties. *Journal of Mathematical Chemistry*, 56 (2):449–476, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0803-3`.

Cassidy:2018:CEA

[2817] Tyler Cassidy, Philippe Gaudreau, and Hassan Safouhi. On the computation of eigenvalues of the anharmonic Coulombic potential. *Journal of Mathematical Chemistry*, 56(2):477–492, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0801-5`. See comment [3010].

Pupyshev:2018:MCS

[2818] Vladimir I. Pupyshev and H. E. Montgomery, Jr. Monotonicity in confined system problems. *Journal of Mathematical Chemistry*, 56(2): 493–507, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0797-x`.

Murugan:2018:TRE

[2819] R. Murugan. Theory on the rate equation of Michaelis–Menten type single-substrate enzyme catalyzed reactions. *Journal of Mathematical Chemistry*, 56(2):508–556, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0791-3`.

Fernandez:2018:SFP

[2820] Francisco M. Fernández. On the symmetry of four particles in a one-dimensional box with harmonic interaction. *Journal of Mathematical Chemistry*, 56(2):557–567, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0800-6`.

Zhang:2018:AIC

[2821] Xiu-Mei Zhang, Yu-Qin Sun, Hua Wang, and Xiao-Dong Zhang. On the ABC index of connected graphs with given degree sequences. *Journal of Mathematical Chemistry*, 56(2):568–582, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0802-4`.

Stamov:2018:APP

[2822] Gani Stamov and Ivanka Stamova. On almost periodic processes in impulsive fractional-order competitive systems. *Journal of Mathematical Chemistry*, 56(2):583–596, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0805-1`.

Berczi-Kovacs:2018:CCN

[2823] Erika R. Bérczi-Kovács and Attila Bernáth. The complexity of the Clar number problem and an exact algorithm. *Journal of Mathematical Chemistry*, 56(2):597–605, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0799-8`.

Furuya:2018:DRM

[2824] Michitaka Furuya, Masanori Takatou, and Shoichi Tsuchiya. Distance-restricted matching extendability of fullerene graphs. *Journal of Mathematical Chemistry*, 56(2):606–617, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0806-0`.

Camby:2018:EDB

[2825] E. Camby, G. Caporossi, M. H. M. Paiva, and M. E. V. Segatto. Expected distance based on random walks. *Journal of Mathematical Chemistry*, 56 (2):618–629, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0808-y`.

Frolov:2018:BFE

[2826] Alexei M. Frolov and David M. Wardlaw. Bremsstrahlung from few-electron ions. *Journal of Mathematical Chemistry*, 56(2):630–649, February 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0798-9`.

Bucknum:2018:SFS

[2827] Michael J. Bucknum and Eduardo A. Castro. Sommerfeld's fine structure constant approximated as a series representation in e and π. *Journal of Mathematical Chemistry*, 56(3):651–655, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0835-8`.

Berg:2018:NMF

[2828] Dmitriy B. Berg and T. E. Simos. A new multistep finite difference pair for the Schrödinger equation and related problems. *Journal of Mathematical Chemistry*, 56(3):656–686, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0812-2`.

Ayala-Hernandez:2018:MMP

[2829] L. E. Ayala-Hernández, Armando Gallegos, J. E. Macías-Díaz, M. L. Miranda-Beltrán, and H. Vargas-Rodríguez. A mathematical model for the pre-diagnostic of glioma growth based on blood glucose levels. *Journal of Mathematical Chemistry*, 56(3):687–699, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0821-1`.

Tikhonov:2018:MMS

[2830] N. A. Tikhonov. Mathematical modeling of solution deionization by sorption on aerogel electrodes. *Journal of Mathematical Chemistry*, 56 (3):700–712, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0825-x`.

Huang:2018:IVI

[2831] Xin Huang, Yi-Ping Luo, Qing-Song Xu, and Yi-Zeng Liang. Incorporating variable importance into kernel PLS for modeling the structure-activity relationship. *Journal of Mathematical Chemistry*, 56(3):713–727, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0826-9`.

Basilevsky:2018:CCM

[2832] Mikhail V. Basilevsky and Sergey V. Titov. The charge-carrier mobility in disordered organic materials: the long-range one-dimensional diffusion with the memory effect. *Journal of Mathematical Chemistry*, 56 (3):728–746, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0827-8`.

Gundogar:2018:BTM

[2833] Zeynep Gündogar and Metin Demiralp. Block tridiagonal matrix enhanced multivariance products representation (BTMEMPR). *Journal*

of Mathematical Chemistry, 56(3):747–769, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0828-7`.

Zheng:2018:NTS

[2834] Jinbin Zheng, Chenglian Liu, and T. E. Simos. A new two-step finite difference pair with optimal properties. *Journal of Mathematical Chemistry*, 56(3):770–798, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0829-6`.

Yang:2018:MTD

[2835] Yanping Yang, Yonglei Fang, and Xiong You. Modified two-derivative Runge–Kutta methods for the Schrödinger equation. *Journal of Mathematical Chemistry*, 56(3):799–812, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0830-0`.

Ohta:2018:CVP

[2836] Katsuhisa Ohta. Constraints in the variational principle for stationary states. *Journal of Mathematical Chemistry*, 56(3):813–824, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0832-y`.

Awonusika:2018:SFR

[2837] Richard Olu Awonusika. Special function representations of the Poisson kernel on hyperbolic spaces. *Journal of Mathematical Chemistry*, 56 (3):825–849, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0833-x`.

Turulski:2018:BSS

[2838] Jan Turulski. Binary self-similar chemical structures. *Journal of Mathematical Chemistry*, 56(3):850–863, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0834-9`.

Valko:2018:IEC

[2839] É. Valkó, T. Varga, A. S. Tomlin, Á. Busai, and T. Turányi. Investigation of the effect of correlated uncertain rate parameters via the calculation of global and local sensitivity indices. *Journal of Mathematical Chemistry*, 56(3):864–889, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0836-7.

Strekalov:2018:QTE

[2840] Mikhail L. Strekalov. Quantum tunneling in an exactly solvable double-barrier potential: barrier transmission near the zero energy. *Journal of Mathematical Chemistry*, 56(3):890–903, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0838-5.

Din:2018:BAC

[2841] Qamar Din. Bifurcation analysis and chaos control in discrete-time glycolysis models. *Journal of Mathematical Chemistry*, 56(3):904–931, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0839-4.

Belkic:2018:EEA

[2842] Dzevad Belkić and Karen Belkić. Explicit extraction of absorption peak positions, widths and heights using higher order derivatives of total shape spectra by nonparametric processing of time signals as complex damped multi-exponentials. *Journal of Mathematical Chemistry*, 56(3):932–977, March 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0852-7; https://link.springer.com/content/pdf/10.1007/s10910-017-0852-7.pdf.

Carbo-Dorca:2018:TSE

[2843] Ramon Carbó-Dorca. Thermal scaling of electronic energy expressions. *Journal of Mathematical Chemistry*, 56(4):979–981, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0864-y.

Shi:2018:NFS

[2844] Xin Shi and T. E. Simos. New five-stages finite difference pair with optimized phase properties. *Journal of Mathematical Chemistry*, 56(4):982–1010, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0831-z.

Diaz-Alvarado:2018:SRP

[2845] Felipe A. Díaz-Alvarado, Jenny Miranda-Pérez, and Ignacio E. Grossmann. Search for reaction pathways with p-graphs and reaction blocks:

methanation of carbon dioxide with hydrogen. *Journal of Mathematical Chemistry*, 56(4):1011–1102, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0844-7`.

Tratnik:2018:GPI

[2846] Niko Tratnik and Petra Zigert Pletersek. The Graovac–Pisanski index of armchair tubulenes. *Journal of Mathematical Chemistry*, 56(4): 1103–1116, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0846-5`.

Liu:2018:AEH

[2847] Shiwei Liu, Juan Zheng, Yonglei Fang, and Xiong You. An adapted explicit hybrid four-step method for the numerical solution of perturbed oscillators. *Journal of Mathematical Chemistry*, 56(4):1117–1129, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0842-9`.

Ehigie:2018:EFS

[2848] Julius Osato Ehigie, Dongxu Diao, Ruqiang Zhang, Yonglei Fang, Xilin Hou, and Xiong You. Exponentially fitted symmetric and symplectic DIRK methods for oscillatory Hamiltonian systems. *Journal of Mathematical Chemistry*, 56(4):1130–1152, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0841-x`.

Kram:2018:AEK

[2849] Sebastian Kram, Maximilian Schäfer, and Rudolf Rabenstein. Approximation of enzyme kinetics for high enzyme concentration by a first order perturbation approach. *Journal of Mathematical Chemistry*, 56(4): 1153–1183, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0848-3`.

Myland:2018:JEF

[2850] Jan C. Myland and Keith B. Oldham. Jacobian elliptic functions describe the properties of the diffuse charge region in narrow electrochemical cells. *Journal of Mathematical Chemistry*, 56(4):1184–1205, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0847-4`.

Medvedev:2018:NSS

[2851] Maxim A. Medvedev and T. E. Simos. A new six-step algorithm with improved properties for the numerical solution of second order initial and/or boundary value problems. *Journal of Mathematical Chemistry*, 56 (4):1206–1233, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0840-y`.

Jiang:2018:EFD

[2852] Xiaoyu Jiang and Kicheon Hong. Explicit form of determinants and inverse matrices of Tribonacci r-circulant type matrices. *Journal of Mathematical Chemistry*, 56(4):1234–1249, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0843-8`.

Zhang:2018:TFM

[2853] Yanwei Zhang, Yonglei Fang, Xiong You, and Guangde Liu. Trigonometrically-fitted multi-derivative linear methods for the resonant state of the Schrödinger equation. *Journal of Mathematical Chemistry*, 56(4):1250–1261, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0851-8`.

Xia:2018:TMO

[2854] Qingyuan Xia and Hui Liu. A theoretical method for obtaining Padé type approximation to temperature integrals via the Stieltjes integral. *Journal of Mathematical Chemistry*, 56(4):1262–1279, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0845-6`.

Medvedev:2018:NTS

[2855] Maxim A. Medvedev and T. E. Simos. A new three-stages six-step finite difference pair with optimal phase properties for second order initial and/or boundary value problems with periodical and/or oscillating solutions. *Journal of Mathematical Chemistry*, 56(4):1280–1312, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0850-9`.

Liu:2018:FSS

[2856] Chenglian Liu and T. E. Simos. A five-stages symmetric method with improved phase properties. *Journal of Mathematical Chemistry*, 56(4): 1313–1338, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0853-6.

Quapp:2018:MMF

[2857] Wolfgang Quapp. A minimal 2D model of the free energy surface for a unidirectional natural molecular motor. *Journal of Mathematical Chemistry*, 56(4):1339–1347, April 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0861-1.

Carbo-Dorca:2018:BHT

[2858] Ramon Carbó-Dorca. Boolean hypercubes as time representation holders. *Journal of Mathematical Chemistry*, 56(5):1349–1352, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0865-x.

Carbo-Dorca:2018:DUB

[2859] Ramon Carbó-Dorca. DNA, unnatural base pairs and hypercubes. *Journal of Mathematical Chemistry*, 56(5):1353–1356, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0866-9.

Carbo-Dorca:2018:ATV

[2860] Ramon Carbó-Dorca. Atomic thermal voltage population distributions. *Journal of Mathematical Chemistry*, 56(5):1357–1359, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0869-6.

Bucknum:2018:AEP

[2861] Michael J. Bucknum and Eduardo A. Castro. Approximation of the electron-proton mass ratio as a series in powers of π. *Journal of Mathematical Chemistry*, 56(5):1360–1364, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0872-y.

Ferrari:2018:DFD

[2862] Margherita Maria Ferrari, Anna Cook, Alana Houlihan, Rebecca Rouleau, Nadrian C. Seeman, Greta Pangborn, and Joanna Ellis-Monaghan. Design formalism for DNA self-assembly of polyhedral skeletons using rigid tiles. *Journal of Mathematical Chemistry*, 56(5):1365–1392, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0858-9.

Langner:2018:AGG

[2863] Johanna Langner and Henryk A. Witek. Algorithm for generating generalized resonance structures of single zigzag chains based on interface theory. *Journal of Mathematical Chemistry*, 56(5):1393–1406, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0860-2`.

Mackay:2018:PAS

[2864] Don Mackay, Jan C. Myland, Keith B. Oldham, and J. Mark Parnis. Pitfalls in the application of statistics to chemical data: the determination of the partition ratio K_{ow} as a case in point. *Journal of Mathematical Chemistry*, 56(5):1407–1427, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0862-0`.

Perez:2018:GCS

[2865] Thomas Perez and Patrick Cassam-Chenaï. Generalization of the concepts of seniority number and ionicity. *Journal of Mathematical Chemistry*, 56(5):1428–1436, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0863-z`.

Brinkmann:2018:CMC

[2866] Gunnar Brinkmann. Computing the maximal canonical form for trees in polynomial time. *Journal of Mathematical Chemistry*, 56(5):1437–1444, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0867-8`.

Mitxelena:2018:ASO

[2867] Ion Mitxelena and Mario Piris. Analytic second-order energy derivatives in natural orbital functional theory. *Journal of Mathematical Chemistry*, 56(5):1445–1455, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0870-0`.

Tsitouras:2018:NEO

[2868] Ch. Tsitouras and I. Th. Famelis. A new eighth order exponentially fitted explicit Numerov-type method for solving oscillatory problems. *Journal of Mathematical Chemistry*, 56(5):1456–1466, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0873-x`.

Pandey:2018:INN

[2869] Pradumn Kumar Pandey, Bibhas Adhikari, and Jayanta Chakraborty. Interpreting nucleation as a network formation process. *Journal of Mathematical Chemistry*, 56(5):1467–1480, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0875-8`.

Gao:2018:TDO

[2870] Yingying Gao, Enqiang Zhu, Zehui Shao, Ivan Gutman, and Antoaneta Klobučar. Total domination and open packing in some chemical graphs. *Journal of Mathematical Chemistry*, 56(5):1481–1492, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0877-6`.

Arockiaraj:2018:HWW

[2871] Micheal Arockiaraj, S. Ruth Julie Kavitha, Krishnan Balasubramanian, and Ivan Gutman. Hyper-Wiener and Wiener polarity indices of silicate and oxide frameworks. *Journal of Mathematical Chemistry*, 56(5): 1493–1510, May 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0881-x`.

Fernandez:2018:CKE

[2872] Francisco M. Fernández. Comment on: "The kinetic energy partition method applied to quantum eigenvalue problems with many harmonic-oscillator potentials" by Y.-H. Chen and S. D. Chao. *Journal of Mathematical Chemistry*, 56(6):1511–1514, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0884-7`. See [2751].

Celebre:2018:AAW

[2873] Giorgio Celebre. An analytical altitude- and wavelength-dependent expression of the j_3 rate coefficient governing the photolysis of the atmospheric ozone. *Journal of Mathematical Chemistry*, 56(6):1515–1519, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0892-7`.

Milani:2018:RBK

[2874] G. Milani and F. Milani. Rubber blends: kinetic numerical model by rheometer experimental characterization. *Journal of Mathematical*

Chemistry, 56(6):1520–1542, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0887-4`.

Alqahtani:2018:NSS

[2875] Aisha M. Alqahtani. Numerical simulation to study the pattern formation of reaction-diffusion Brusselator model arising in triple collision and enzymatic. *Journal of Mathematical Chemistry*, 56(6):1543–1566, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0859-8`.

Yao:2018:NFS

[2876] Junfeng Yao and T. E. Simos. New five-stages two-step method with improved characteristics. *Journal of Mathematical Chemistry*, 56(6):1567–1594, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0874-9`.

Paldus:2018:VBA

[2877] Josef Paldus and Josep Planelles. Valence bond approach and Verma bases. *Journal of Mathematical Chemistry*, 56(6):1595–1630, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0876-7`.

Dharmani:2018:MGG

[2878] Bhaveshkumar C. Dharmani. Multivariate generalized Gram–Charlier series in vector notations. *Journal of Mathematical Chemistry*, 56(6):1631–1655, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0878-5`.

Boumali:2018:SPD

[2879] Abdelmalek Boumali. The statistical properties of q-deformed Morse potential for some diatomic molecules via Euler–MacLaurin method in one dimension. *Journal of Mathematical Chemistry*, 56(6):1656–1666, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0879-4`.

Verma:2018:CMT

[2880] Amit Kumar Verma and Sheerin Kayenat. On the convergence of Mickens' type nonstandard finite difference schemes on Lane–Emden

type equations. *Journal of Mathematical Chemistry*, 56(6):1667–1706, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0880-y. See correction [3014].

Wang:2018:PHM

[2881] Li Wang, Bernhard Maschke, and Arjan van der Schaft. Port-Hamiltonian modeling of non-isothermal chemical reaction networks. *Journal of Mathematical Chemistry*, 56(6):1707–1727, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0882-9; https://link.springer.com/content/pdf/10.1007/s10910-018-0882-9.pdf.

Katz:2018:TCP

[2882] Jordan Katz and Diana Hubbard. A topological characterization of the products arising from site-specific recombination on $T(2,n)\#C(2,r)$ DNA substrates. *Journal of Mathematical Chemistry*, 56(6):1728–1743, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0883-8.

Zhai:2018:PSS

[2883] Xiuyun Zhai, Mingtong Chen, Wencong Lu, and Dongping Chang. Predicting specific surface areas of layered double hydroxides based on support vector regression integrated with a residual bootstrapping method. *Journal of Mathematical Chemistry*, 56(6):1744–1758, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0889-2.

Frank:2018:QSS

[2884] Martin Frank, Christian Lax, Sebastian Walcher, and Olaf Wittich. Quasi-steady state reduction for the Michaelis–Menten reaction-diffusion system. *Journal of Mathematical Chemistry*, 56(6):1759–1781, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0891-8.

Agreda:2018:LAB

[2885] Jesús Ágreda, Carolina Mejía, and J. Andrés Montoya. On the linear algebra of biological homochirality. *Journal of Mathematical Chemistry*, 56(6):1782–1810, June 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0893-6.

Aguiar:2018:FSI

[2886] Jesús Vigo Aguiar. Foreword for the special issue on CMMSE 2017. *Journal of Mathematical Chemistry*, 56(7):1811–1812, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0923-4; https://link.springer.com/content/pdf/10.1007/s10910-018-0923-4.pdf`.

Bayon:2018:CGA

[2887] L. Bayón, P. Fortuny Ayuso, J. M. Grau, M. M. Ruiz, and P. M. Suárez. CMMSE-17: general analytical laws for metabolic pathways. *Journal of Mathematical Chemistry*, 56(7):1813–1825, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0810-4`.

Gozukirmizi:2018:PET

[2888] Cosar Gözükirmizi and Metin Demiralp. Probabilistic evolution theory for explicit autonomous ordinary differential equations: recursion of squarified telescope matrices and optimal space extension. *Journal of Mathematical Chemistry*, 56(7):1826–1848, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0849-2`.

Rodriguez:2018:CFG

[2889] José M. Rodríguez, José L. Sánchez, and José M. Sigarreta. CMMSE — on the first general Zagreb index. *Journal of Mathematical Chemistry*, 56(7):1849–1864, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0816-y`.

Martinez-Perez:2018:CNA

[2890] Alvaro Martínez-Pérez, José M. Rodríguez, and José M. Sigarreta. CMMSE: A new approximation to the geometric–arithmetic index. *Journal of Mathematical Chemistry*, 56(7):1865–1883, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0811-3`.

Zafar:2018:OIM

[2891] Fiza Zafar, Alicia Cordero, R. Quratulain, and Juan R. Torregrosa. Optimal iterative methods for finding multiple roots of nonlinear equations using free parameters. *Journal of Mathematical Chemistry*, 56(7):1884–1901, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0813-1.

Cordero:2018:CTC

[2892] Alicia Cordero, Lucía Guasp, and Juan R. Torregrosa. CMMSE2017: On two classes of fourth- and seventh-order vectorial methods with stable behavior. *Journal of Mathematical Chemistry*, 56(7):1902–1923, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0814-0.

Fang:2018:TDR

[2893] Yonglei Fang, Yanwei Zhang, and Ping Wang. Two-derivative Runge–Kutta methods with increased phase-lag and dissipation order for the Schrödinger equation. *Journal of Mathematical Chemistry*, 56(7):1924–1934, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0817-x.

Magrenan:2018:SLM

[2894] Á. Alberto Magreñán, Ioannis K. Argyros, Lara Orcos, and Juan Antonio Sicilia. Secant-like methods for solving nonlinear models with applications to chemistry. *Journal of Mathematical Chemistry*, 56(7):1935–1957, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0824-y.

Argyros:2018:ISC

[2895] Ioannis K. Argyros, Elena Giménez, Á. A. Magreñán, Í. Sarría, and Juan Antonio Sicilia. Improved semilocal convergence analysis in Banach space with applications to chemistry. *Journal of Mathematical Chemistry*, 56(7):1958–1975, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0823-z.

Macias-Diaz:2018:TWS

[2896] Jorge E. Macías-Díaz and Héctor Vargas-Rodríguez. Traveling-wave solutions of a generalized damped wave equation with time-dependent coefficients through the trial equation method. *Journal of Mathematical Chemistry*, 56(7):1976–1984, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-017-0819-8.

Macias-Diaz:2018:SPC

[2897] Jorge E. Macías-Díaz and Armando Gallegos. A structure-preserving computational method in the simulation of the dynamics of cancer growth with radiotherapy. *Journal of Mathematical Chemistry*, 56(7): 1985–2000, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0818-9`.

Demiralp:2018:PER

[2898] Metin Demiralp. Promenading in the enchanted realm of Kronecker powers: single monomial probabilistic evolution theory (PREVTH) in evolver dynamics. *Journal of Mathematical Chemistry*, 56(7):2001–2023, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0822-0`.

Kalay:2018:SEP

[2899] Berfin Kalay and Metin Demiralp. Somehow emancipating Probabilistic Evolution Theory (PREVTH) from singularities via getting single monomial PREVTH. *Journal of Mathematical Chemistry*, 56(7): 2024–2043, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-017-0815-z`.

Ozdemir:2018:UEF

[2900] Semra Bayat Özdemir and Metin Demiralp. Using enchanted features of Constancy Adding Space Extension (CASE) to reduce the dimension of evolver dynamics: Single Monomial Probabilistic Evolution Theory. *Journal of Mathematical Chemistry*, 56(7):2044–2068, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0854-0`.

Behl:2018:OSM

[2901] Ramandeep Behl, Ali Saleh Alshomrani, and S. S. Motsa. An optimal scheme for multiple roots of nonlinear equations with eighth-order convergence. *Journal of Mathematical Chemistry*, 56(7):2069–2084, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0857-x`.

Garcia:2018:EAS

[2902] Gonzalo Cerruela García, Nicolás García-Pedrajas, Irene Luque Ruiz, and Miguel Ángel Gómez-Nieto. An ensemble approach for in silico pre-

diction of Ames mutagenicity. *Journal of Mathematical Chemistry*, 56(7): 2085–2098, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0855-z`.

Maroju:2018:SDF

[2903] P. Maroju, Á. A. Magreñán, S. S. Motsa, and Í. Sarría. Second derivative free sixth order continuation method for solving nonlinear equations with applications. *Journal of Mathematical Chemistry*, 56(7): 2099–2116, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0868-7`.

Magrenan:2018:BCS

[2904] Á. A. Magreñán, I. K. Argyros, J. J. Rainer, and J. A. Sicilia. Ball convergence of a sixth-order Newton-like method based on means under weak conditions. *Journal of Mathematical Chemistry*, 56(7):2117–2131, August 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0856-y`.

Belkic:2018:ELF

[2905] Dzevad Belkić. The Euler T and Lambert W functions in mechanistic radiobiological models with chemical kinetics for repair of irradiated cells. *Journal of Mathematical Chemistry*, 56(8):2133–2193, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0932-3; https://link.springer.com/content/pdf/10.1007/s10910-018-0932-3.pdf`.

Balasubramanian:2018:RJT

[2906] Krishnan Balasubramanian. Relativity and the Jahn–Teller, Berry pseudorotations of TBP clusters: group theory, spin-orbit and combinatorial nuclear spin statistics of TBP Desargues–Levi isomerization graph. *Journal of Mathematical Chemistry*, 56(8):2194–2225, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0885-6`.

Fujita:2018:HEK

[2907] Shinsaku Fujita. Hierarchical enumeration of Kekulé's benzenes, Ladenburg's benzenes, Dewar's benzenes, and benzvalenes by using combined-permutation representations. *Journal of Mathematical Chemistry*, 56(8): 2226–2266, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0886-5.

Alolyan:2018:NTS

[2908] Ibraheem Alolyan and T. E. Simos. New three-stages symmetric six-step finite difference method with vanished phase-lag and its derivatives up to sixth derivative for second order initial and/or boundary value problems with periodical and/or oscillating solutions. *Journal of Mathematical Chemistry*, 56(8):2267–2301, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0888-3.

Kovalnogov:2018:NHT

[2909] V. N. Kovalnogov, R. V. Fedorov, A. A. Bondarenko, and T. E. Simos. New hybrid two-step method with optimized phase and stability characteristics. *Journal of Mathematical Chemistry*, 56(8):2302–2340, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0894-5.

Krajnak:2018:PSG

[2910] Vladimír Krajnák and Holger Waalkens. The phase space geometry underlying roaming reaction dynamics. *Journal of Mathematical Chemistry*, 56(8):2341–2378, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0895-4; https://link.springer.com/content/pdf/10.1007/s10910-018-0895-4.pdf.

Rinderspacher:2018:CCD

[2911] B. Christopher Rinderspacher. Chemical compound design using nuclear charge distributions. *Journal of Mathematical Chemistry*, 56(8):2379–2391, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0896-3.

Yau:2018:MME

[2912] Ching Koon Yau and Christopher G. Jesudason. Mathematical modeling of the effects of attenuation and system electronic coupling on the determination of speed of sound in ultrasonic interferometry. *Journal of Mathematical Chemistry*, 56(8):2392–2417, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0897-2.

Kipriyanov:2018:BNM

[2913] Alexey A. Kipriyanov, Alexander A. Kipriyanov, and Alexander B. Doktorov. Binary non-Markovian theory of bulk associative-dissociative reaction $A + A \leftrightarrow C$. I: many-particle aspects of the theory. *Journal of Mathematical Chemistry*, 56(8):2418–2453, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0898-1`.

Yan:2018:NRK

[2914] Ke Yan and T. E. Simos. New Runge–Kutta type symmetric two-step method with optimized characteristics. *Journal of Mathematical Chemistry*, 56(8):2454–2484, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0899-0`.

Mushtaq:2018:CAS

[2915] Qaiser Mushtaq and Nighat Mumtaz. PSL$(2, 7)$ and carbon allotrope D 168 Schwarzite. *Journal of Mathematical Chemistry*, 56(8):2485–2494, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0900-y`. See correction [2916].

Mushtaq:2018:CPC

[2916] Qaiser Mushtaq and Nighat Mumtaz. Correction to: PSL$(2, 7)$ and carbon allotrope D 168 Schwarzite. *Journal of Mathematical Chemistry*, 56(8):2495, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0903-8; https://link.springer.com/content/pdf/10.1007/s10910-018-0903-8.pdf`. See [2915].

Li:2018:SRC

[2917] Hui Li, Shuqin Jia, Tianliang Zhao, and Ying Huai. Skeletal and reduced chemical mechanism for hydrogen fluoride chemical laser. *Journal of Mathematical Chemistry*, 56(8):2496–2511, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0901-x`.

Doslic:2018:PEA

[2918] Tomislav Doslić and Ivana Zubac. Partition of π-electrons among the faces of polyhedral carbon clusters. *Journal of Mathematical Chemistry*, 56(8):2512–2524, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0902-9`.

Zhao:2018:SME

[2919] Yun Zhao, Jianfeng He, and Jing Li. The structural modeling of EF-hand motifs in parvalbumin. *Journal of Mathematical Chemistry*, 56(8):2525–2536, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0904-7`.

Belkic:2018:VRC

[2920] Dzevad Belkić and Karen Belkić. Validation of reconstructed component spectra from non-parametric derivative envelopes: comparison with component lineshapes from parametric derivative estimations with the solved quantification problem. *Journal of Mathematical Chemistry*, 56 (8):2537–2578, September 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0906-5; https://link.springer.com/content/pdf/10.1007/s10910-018-0906-5.pdf`.

Singh:2018:OHA

[2921] Randhir Singh. Optimal homotopy analysis method for the non-isothermal reaction-diffusion model equations in a spherical catalyst. *Journal of Mathematical Chemistry*, 56(9):2579–2590, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0911-8`.

Chen:2018:NTS

[2922] Zhong Chen, Chenglian Liu, and T. E. Simos. New three-stages symmetric two step method with improved properties for second order initial/boundary value problems. *Journal of Mathematical Chemistry*, 56(9): 2591–2616, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0905-6`.

Elyukhina:2018:GNP

[2923] Inna Elyukhina. 2D general nonlinear parabolic equation for unstable wave package envelope in structural macrokinetics. *Journal of Mathematical Chemistry*, 56(9):2617–2625, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0907-4`.

Skakauskas:2018:MNC

[2924] V. Skakauskas, P. Katauskis, and R. Ciegis. Modelling of the NO + CO reaction over inhomogeneous surfaces. *Journal of Mathematical Chem-*

istry, 56(9):2626–2642, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0908-3`.

Mendoza:2018:PEW

[2925] Eduardo R. Mendoza, Dylan Antonio S. J. Talabis, and Editha C. Jose. Positive equilibria of weakly reversible power law kinetic systems with linear independent interactions. *Journal of Mathematical Chemistry*, 56(9):2643–2673, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0909-2; https://link.springer.com/content/pdf/10.1007/s10910-018-0909-2.pdf`.

Thylwe:2018:HPR

[2926] Karl-Erik Thylwe. Heavy-particle resonance phase shifts: an improved amplitude-phase formula. *Journal of Mathematical Chemistry*, 56(9):2674–2690, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0910-9; https://link.springer.com/content/pdf/10.1007/s10910-018-0910-9.pdf`.

Hao:2018:EMS

[2927] Tian-Chu Hao, Fu-Zhong Cong, and Yu-Feng Shang. An efficient method for solving coupled Lane–Emden boundary value problems in catalytic diffusion reactions and error estimate. *Journal of Mathematical Chemistry*, 56(9):2691–2706, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0912-7`.

Balasubramanian:2018:CMG

[2928] Krishnan Balasubramanian. Combinatorial multinomial generators for colorings of 4D-hypercubes and their applications. *Journal of Mathematical Chemistry*, 56(9):2707–2723, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0913-6`.

Yang:2018:CEA

[2929] Zhen Yang, Xingsheng Gu, Changjian Ling, and Xiaoyi Liang. Computational and experimental approaches for investigating membranes diffusion behavior in model diesel fuel. *Journal of Mathematical Chemistry*, 56(9):2724–2740, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0914-5`.

Stasinos:2018:NSS

[2930] P. I. Stasinos and Theodore E. Simos. New 8-step symmetric embedded predictor-corrector (EPCM) method with vanished phase-lag and its first derivative for the numerical integration of the Schrödinger equation. *Journal of Mathematical Chemistry*, 56(9):2741–2767, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0915-4`.

Zhao:2018:CSV

[2931] Chang Zhao, Yi Fu Li, Bao Qiang Xu, Bin Yang, Da Chun Liu, and Hong Wei Yang. Calculation of the second virial coefficients of alkali metals by modified Peng–Robinson equation. *Journal of Mathematical Chemistry*, 56(9):2768–2784, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0916-3`.

Sun:2018:BFG

[2932] Chunhu Sun and Heping Zhang. On bicriticality of (3,6)-fullerene graphs. *Journal of Mathematical Chemistry*, 56(9):2785–2793, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0917-2`.

Doslic:2018:NST

[2933] Tomislav Doslić. On the number of spanning trees in alternating polycyclic chains. *Journal of Mathematical Chemistry*, 56(9):2794–2800, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0918-1`.

Andova:2018:DBIa

[2934] Vesna Andova, Martin Knor, and Riste Skrekovski. Distance based indices in nanotubical graphs: part 1. *Journal of Mathematical Chemistry*, 56(9):2801–2815, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0919-0`.

Kovalnogov:2018:NHS

[2935] V. N. Kovalnogov, R. V. Fedorov, and T. E. Simos. New hybrid symmetric two step scheme with optimized characteristics for second order problems. *Journal of Mathematical Chemistry*, 56(9):2816–2844, October 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0920-7`.

Fujita:2018:HEO

[2936] Shinsaku Fujita. Hierarchical enumeration of octahedral complexes by using combined-permutation representations. *Journal of Mathematical Chemistry*, 56(10):2845–2875, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0921-6`.

DAmbrosio:2018:ANM

[2937] Raffaele D'Ambrosio, Martina Moccaldi, Beatrice Paternoster, and Federico Rossi. Adapted numerical modelling of the Belousov–Zhabotinsky reaction. *Journal of Mathematical Chemistry*, 56(10):2876–2897, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0922-5`.

Alolyan:2018:NFS

[2938] Ibraheem Alolyan and T. E. Simos. New four-stages symmetric six-step method with improved phase properties for second order problems with periodical and/or oscillating solutions. *Journal of Mathematical Chemistry*, 56(10):2898–2928, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0924-3`.

Fortun:2018:DOA

[2939] Noel T. Fortun, Eduardo R. Mendoza, Luis F. Razon, and Angelyn R. Lao. A deficiency–one algorithm for power-law kinetic systems with reactant-determined interactions. *Journal of Mathematical Chemistry*, 56(10):2929–2962, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0925-2`.

Alexander:2018:IUS

[2940] M. Vijay Alexander and G. Meenakshi. Investigation of ultrasonic speeds of sound and excess parameters in binary liquid mixtures of N-alkanes with octan-2-ol using different empirical theories at 298.15 K. *Journal of Mathematical Chemistry*, 56(10):2963–2981, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0926-1`.

Liu:2018:SKG

[2941] Han-Bin Liu, Liang-Zhong Yi, and Chun-Sheng Jia. Solutions of the Klein–Gordon equation with the improved Tietz potential energy model. *Journal of Mathematical Chemistry*, 56(10):2982–2994, November 2018.

CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0927-0.

Doslic:2018:MI

[2942] Tomislav Došlić, Ivica Martinjak, Riste Škrekovski, Sanja Tipurić Spužević, and Ivana Zubac. Mostar index. *Journal of Mathematical Chemistry*, 56(10):2995–3013, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0928-z.

Hao:2018:NRK

[2943] Ruru Hao and T. E. Simos. New Runge–Kutta type symmetric two step finite difference pair with improved properties for second order initial and/or boundary value problems. *Journal of Mathematical Chemistry*, 56(10):3014–3044, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0930-5.

Din:2018:NCC

[2944] Qamar Din. A novel chaos control strategy for discrete-time Brusselator models. *Journal of Mathematical Chemistry*, 56(10):3045–3075, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0931-4.

Andova:2018:DBIb

[2945] Vesna Andova, Martin Knor, and Riste Skrekovski. Distance based indices in nanotubical graphs: part 2. *Journal of Mathematical Chemistry*, 56(10):3076–3088, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0933-2.

Meral:2018:MAN

[2946] Gülnihal Meral and Neslihan Nesliye Pelen. Mathematical analysis and numerical simulations for the HSP70 synthesis model. *Journal of Mathematical Chemistry*, 56(10):3089–3114, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0934-1.

He:2018:EFD

[2947] Jianfeng He, Yun Zhao, and Jing Li. The ensemble folding dynamics of EF-hand domain in parvalbumin from a Monte Carlo simulation. *Journal of Mathematical Chemistry*, 56(10):3115–3125, November 2018. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0935-0.

Sakiyama:2018:ECO

[2948] Hiroshi Sakiyama and Katsushi Waki. Enumeration of conformers for octahedral trans/cis-[MX_2 $(AB)_4$] and trans/cis-[MX_2 $(ABC)_4$] complexes on the basis of computational group theory. *Journal of Mathematical Chemistry*, 56(10):3126–3135, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0936-z.

Huang:2018:HIM

[2949] Yufeng Huang, Lingsheng Shi, and Xingyu Xu. The Hosoya index and the Merrifield–Simmons index. *Journal of Mathematical Chemistry*, 56(10):3136–3146, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0937-y; https://link.springer.com/content/pdf/10.1007/s10910-018-0937-y.pdf.

Wang:2018:PPK

[2950] Yan Wang. Pfaffian polyominos on the Klein bottle. *Journal of Mathematical Chemistry*, 56(10):3147–3160, November 2018. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0938-x.

Belkic:2019:DCE

[2951] Dzevad Belkić. Double charge exchange in ion-atom collisions using distorted wave theories with two-electron continuum intermediate states in one or both scattering channels. *Journal of Mathematical Chemistry*, 57(1):1–58, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0967-5; https://link.springer.com/content/pdf/10.1007/s10910-018-0967-5.pdf.

Belkic:2019:ATR

[2952] Dzevad Belkić. All the trinomial roots, their powers and logarithms from the Lambert series, Bell polynomials and Fox–Wright function: illustration for genome multiplicity in survival of irradiated cells. *Journal of Mathematical Chemistry*, 57(1):59–106, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0985-3; https://link.springer.com/content/pdf/10.1007/s10910-018-0985-3.pdf.

Killingbeck:2019:HDM

[2953] J. P. Killingbeck, G. Jolicard, and A. Grosjean. The Hill determinant method revisited. *Journal of Mathematical Chemistry*, 57(1):107–118, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0939-9; https://link.springer.com/content/pdf/10.1007/s10910-018-0939-9.pdf`.

Qiu:2019:NMM

[2954] Guo-Hua Qiu, Chenglian Liu, and T. E. Simos. A new multistep method with optimized characteristics for initial and/or boundary value problems. *Journal of Mathematical Chemistry*, 57(1):119–148, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0940-3`.

Kumar:2019:NSC

[2955] Sanjay Kumar, Ram Jiwari, and R. C. Mittal. Numerical simulation for computational modelling of reaction-diffusion Brusselator model arising in chemical processes. *Journal of Mathematical Chemistry*, 57(1):149–179, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0941-2`.

Tratnik:2019:EHP

[2956] Niko Tratnik and Petra Zigert Pletersek. The edge-Hosoya polynomial of benzenoid chains. *Journal of Mathematical Chemistry*, 57(1):180–189, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0942-1`.

Trofimov:2019:TLN

[2957] Aleksej Trofimov, Tatjana Gric, and Ortwin Hess. Three-layered nanostructured metamaterials for surface plasmon polariton guiding. *Journal of Mathematical Chemistry*, 57(1):190–201, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0943-0`.

Zhao:2019:FAF

[2958] Shuang Zhao and Heping Zhang. Forcing and anti-forcing polynomials of perfect matchings for some rectangle grids. *Journal of Mathematical Chemistry*, 57(1):202–225, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0944-z`.

Cassam-Chenai:2019:ILB

[2959] P. Cassam-Chenaï. An improved lower bound for the maximal length of a multivector. *Journal of Mathematical Chemistry*, 57(1):226–231, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0947-9`.

Kovalnogov:2019:NMS

[2960] V. N. Kovalnogov, R. V. Fedorov, D. V. Suranov, and T. E. Simos. New multiple stages scheme with improved properties for second order problems. *Journal of Mathematical Chemistry*, 57(1):232–262, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0948-8`.

Hou:2019:IPG

[2961] Yanzhen Hou, Jin Dai, Jianfeng He, Antti J. Niemi, Xubiao Peng, and Nevena Ilieva. Intrinsic protein geometry with application to non-proline cis peptide planes. *Journal of Mathematical Chemistry*, 57(1): 263–279, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0949-7`.

Randic:2019:MCI

[2962] Milan Randić. Mathematical chemistry illustrations: a personal view of less known results. *Journal of Mathematical Chemistry*, 57(1):280–314, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0951-0`.

Tikhonov:2019:PIS

[2963] Nikolay A. Tikhonov. On the phenomenon of isothermal supersaturation of solutions at ion exchange in porous media. *Journal of Mathematical Chemistry*, 57(1):315–326, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0953-y`.

Baronas:2019:CMB

[2964] Romas Baronas, Juozas Kulys, and Linas Petkevicius. Computational modeling of batch stirred tank reactor based on spherical catalyst particles. *Journal of Mathematical Chemistry*, 57(1):327–342, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0954-x`.

Arockiaraj:2019:DBT

[2965] Micheal Arockiaraj, Sandi Klavžar, Shagufa Mushtaq, and Krishnan Balasubramanian. Distance-based topological indices of nanosheets, nanotubes and nanotori of SiO_2. *Journal of Mathematical Chemistry*, 57(1): 343–369, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0956-8`.

Tratnik:2019:FCW

[2966] Niko Tratnik. Formula for calculating the Wiener polarity index with applications to benzenoid graphs and phenylenes. *Journal of Mathematical Chemistry*, 57(1):370–383, January 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0957-7`.

Belkic:2019:RRA

[2967] Dzevad Belkić and Karen Belkić. Review of recent applications of the conventional and derivative fast Padé transform for magnetic resonance spectroscopy. *Journal of Mathematical Chemistry*, 57(2):385–464, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01001-8; https://link.springer.com/content/pdf/10.1007/s10910-019-01001-8.pdf`.

Yao:2019:CCE

[2968] Cui-Xia Yao and Qi-Ying Xia. Coriolis coupling effects in the dynamics of the $D(^2S) + NH(X^3\Sigma^-) \rightarrow N(^4\ S) + H\ D(X^1\Sigma_g^+)$ reaction and its kinetic isotope effect. *Journal of Mathematical Chemistry*, 57(2): 465–472, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0958-6`.

Diudea:2019:RSF

[2969] Mircea V. Diudea and Csaba L. Nagy. Rhombellane space filling. *Journal of Mathematical Chemistry*, 57(2):473–483, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0959-5`.

Koledina:2019:MOO

[2970] K. F. Koledina, S. N. Koledin, A. P. Karpenko, I. M. Gubaydullin, and M. K. Vovdenko. Multi-objective optimization of chemical reaction conditions based on a kinetic model. *Journal of Mathematical Chemistry*, 57

(2):484–493, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0960-z`.

Wang:2019:NMS

[2971] Guiping Wang and T. E. Simos. New multiple stages two-step complete in phase algorithm with improved characteristics for second order initial/boundary value problems. *Journal of Mathematical Chemistry*, 57(2):494–515, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0961-y`.

Kirov:2019:DMP

[2972] Mikhail V. Kirov. Dipole moment of polyhedral water clusters: mathematical relationships and their application. *Journal of Mathematical Chemistry*, 57(2):516–532, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0962-x`.

Komatsu:2019:ASN

[2973] Hirokazu Komatsu, Hiroyuki Nakajima, and Akio Ito. Asymptotic stability of a non-weakly reversible biochemical reaction network composed of cardiac hypertrophy factors. *Journal of Mathematical Chemistry*, 57(2):533–569, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0963-9`.

Madduri:2019:FCI

[2974] Harshita Madduri and Pradip Roul. A fast-converging iterative scheme for solving a system of Lane–Emden equations arising in catalytic diffusion reactions. *Journal of Mathematical Chemistry*, 57(2):570–582, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0964-8`.

Roul:2019:OIA

[2975] Pradip Roul and Harshita Madduri. An optimal iterative algorithm for solving Bratu-type problems. *Journal of Mathematical Chemistry*, 57(2):583–598, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0965-7`.

Bouhank:2019:TMC

[2976] A. Bouhank and L. Bencheikh. Theoretical modelling for calculation of the energy densities of adsorption sites using inverse gas chromatography. *Journal of Mathematical Chemistry*, 57(2):599–608, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0968-4`.

Yurtas:2019:IPZ

[2977] Aysun Yurtas, Muge Togan, Veerebradiah Lokesha, Ismail Naci Cangul, and Ivan Gutman. Inverse problem for Zagreb indices. *Journal of Mathematical Chemistry*, 57(2):609–615, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0970-x`.

Szabo:2019:FAS

[2978] Rebeka Szabó and Gábor Lente. Full analytical solution of a nucleation-growth type kinetic model of nanoparticle formation. *Journal of Mathematical Chemistry*, 57(2):616–631, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0975-5`.

Rech:2019:OPP

[2979] Paulo C. Rech. Organization of the periodicity in the parameter-space of a glycolysis discrete-time mathematical model. *Journal of Mathematical Chemistry*, 57(2):632–637, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0976-4`.

Mvogo:2019:CPF

[2980] Alain Mvogo and Jorge E. Macías-Díaz. Complex pattern formation arising from wave instabilities in a three-agent chemical system with superdiffusion. *Journal of Mathematical Chemistry*, 57(2):638–654, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0977-3`.

Balasubramanian:2019:CMC

[2981] Krishnan Balasubramanian. Computational multinomial combinatorics for colorings of 5D-hypercubes for all irreducible representations and applications. *Journal of Mathematical Chemistry*, 57(2):655–689, February 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0978-2`.

Carbo-Dorca:2019:VSD

[2982] Ramon Carbó-Dorca. Vector spaces defined over the unit interval. *Journal of Mathematical Chemistry*, 57(3):691–693, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00989-9`.

Carbo-Dorca:2019:TBH

[2983] Ramon Carbó-Dorca. Transformation of boolean hypercube vertices into unit interval elements: QSPR workout consequences. *Journal of Mathematical Chemistry*, 57(3):694–696, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00990-2`.

Carbo-Dorca:2019:RSB

[2984] Ramon Carbó-Dorca. Role of the structure of Boolean hypercubes when used as vectors in natural (boolean) vector semispaces. *Journal of Mathematical Chemistry*, 57(3):697–700, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00997-9`.

Khoma:2019:PAC

[2985] Mykhaylo Khoma and Ralph Jaquet. A perturbative approach for the construction of the non-adiabatic nuclear kinetic energy operator for diatomic and triatomic systems. *Journal of Mathematical Chemistry*, 57 (3):701–725, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0979-1`.

Biebighauser:2019:AGR

[2986] Daniel P. Biebighauser and Darin J. Ulness. Application of group ring algebra to localized and delocalized quantum states in periodic potentials. *Journal of Mathematical Chemistry*, 57(3):726–749, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0980-8`.

Saha:2019:WOC

[2987] Sandip Saha and Gautam Gangopadhyay. When an oscillating center in an open system undergoes power law decay. *Journal of Mathematical Chemistry*, 57(3):750–768, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0981-7`.

Yadav:2019:FEA

[2988] Om Prakash Yadav and Ram Jiwari. A finite element approach to capture Turing patterns of autocatalytic Brusselator model. *Journal of Mathematical Chemistry*, 57(3):769–789, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0982-6`.

Pina-Villalpando:2019:NSF

[2989] Luis E. Piña-Villalpando, Jorge E. Macías-Díaz, and Evguenii Kurmyshev. Nonlinear supratransmission in fractional wave systems. *Journal of Mathematical Chemistry*, 57(3):790–811, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0983-5`.

DeBortoli:2019:ORK

[2990] A. L. De Bortoli and F. N. Pereira. Obtaining a reduced kinetic mechanism for methyl butanoate. *Journal of Mathematical Chemistry*, 57 (3):812–833, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0984-4`.

Alolyan:2019:NMS

[2991] Ibraheem Alolyan and T. E. Simos. New multiple stages multistep method with best possible phase properties for second order initial/boundary value problems. *Journal of Mathematical Chemistry*, 57(3): 834–857, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0986-2`.

Sakiyama:2019:TEZ

[2992] Hiroshi Sakiyama. Theoretical equations of Zeeman energy levels for distorted metal complexes with $^5T_{2g}$ ground terms. *Journal of Mathematical Chemistry*, 57(3):858–874, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0987-1`.

Alalwan:2019:TMN

[2993] Najlaa Alalwan, Alex Arenas, and Ernesto Estrada. Topological melting in networks of granular materials. *Journal of Mathematical Chemistry*, 57 (3):875–894, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0988-0`.

Yang:2019:NFS

[2994] Nan Yang and T. E. Simos. New four stages multistep in phase algorithm with best possible properties for second order problems. *Journal of Mathematical Chemistry*, 57(3):895–917, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00991-1`.

Behl:2019:TGH

[2995] Ramandeep Behl, Ali Saleh Alshomrani, and Á. A. Magreñán. Two general higher-order derivative free iterative techniques having optimal convergence order. *Journal of Mathematical Chemistry*, 57(3): 918–938, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00992-0`.

Fernandez:2019:AKP

[2996] Francisco M. Fernández. On the application of the Kronecker product to three-spin systems. *Journal of Mathematical Chemistry*, 57(3): 939–944, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00994-y`.

Roul:2019:NMM

[2997] Pradip Roul. A new mixed MADM–Collocation approach for solving a class of Lane–Emden singular boundary value problems. *Journal of Mathematical Chemistry*, 57(3):945–969, March 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00995-x`.

Fedorov:2019:PCR

[2998] Alexey Alexandrovich Fedorov, Alexander S. Berdnikov, and Vladimir E. Kurochkin. The polymerase chain reaction model analyzed by the homotopy perturbation method. *Journal of Mathematical Chemistry*, 57 (4):971–985, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00998-8`.

Dharmalingam:2019:AES

[2999] K. M. Dharmalingam, M. Veeramuni, and T. Praveen. Analytical expressions of the substrate and mediator of multi-step enzyme electrodes. *Journal of Mathematical Chemistry*, 57(4):986–1000, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL https://link.springer.com/article/10.1007/s10910-019-01003-6.

Ceccato:2019:RMA

[3000] Alessandro Ceccato, Paolo Nicolini, and Diego Frezzato. Recasting the mass-action rate equations of open chemical reaction networks into a universal quadratic format. *Journal of Mathematical Chemistry*, 57(4): 1001–1018, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01005-4.

Milani:2019:NKM

[3001] G. Milani and F. Milani. Numerical kinetic model with regularization for NR–PB natural and poly-butadiene rubber blends: implementation and validation against experimental data. *Journal of Mathematical Chemistry*, 57(4):1019–1034, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01006-3.

Morrison:2019:PSS

[3002] Conor L. Morrison and Bernard Shizgal. Pseudospectral solution of the Schrödinger equation for the Rosen–Morse and Eckart potentials. *Journal of Mathematical Chemistry*, 57(4):1035–1052, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01007-2.

Rodriguez-Velazquez:2019:TNT

[3003] Juan Alberto Rodríguez-Velázquez and Alexandru T. Balaban. Two new topological indices based on graph adjacency matrix eigenvalues and eigenvectors. *Journal of Mathematical Chemistry*, 57(4):1053–1074, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01008-1.

Carbo-Dorca:2019:UTN

[3004] Ramon Carbó-Dorca. Universal transformation and non-linear connection between experimental and calculated property vectors in QSPR. *Journal of Mathematical Chemistry*, 57(4):1075–1087, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01009-0.

Hui:2019:NMT

[3005] Fei Hui and T. E. Simos. New multistage two-step complete in phase scheme with improved properties for quantum chemistry problems. *Journal of Mathematical Chemistry*, 57(4):1088–1111, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01010-7`.

Chen:2019:NMM

[3006] Zhong Chen, Chenglian Liu, Chieh-Wen Hsu, and T. E. Simos. A new multistage multistep full in phase algorithm with optimized characteristics for problems in chemistry. *Journal of Mathematical Chemistry*, 57 (4):1112–1139, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01011-6`.

Ferapontov:2019:ISA

[3007] N. B. Ferapontov, M. G. Tokmachev, S. N. Khudyakova, and Kh. T. Trobov. Influence of the sorbed acids on the swelling degree of the strongly basic ion exchanger. *Journal of Mathematical Chemistry*, 57 (4):1140–1153, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01012-5`.

Mahalakshmi:2019:EWB

[3008] M. Mahalakshmi and G. Hariharan. An efficient wavelet-based method for the numerical solutions of nonlinear coupled reaction-diffusion equations in biochemical engineering. *Journal of Mathematical Chemistry*, 57 (4):1154–1168, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01014-3`.

Bolivar:2019:PSF

[3009] Juan Carlos Bolívar, Ágnes Nagy, and Elvira Romera. Phase-space Fisher information of 2D gapped Dirac materials. *Journal of Mathematical Chemistry*, 57(4):1169–1180, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01015-2; https://link.springer.com/content/pdf/10.1007/s10910-019-01015-2.pdf`.

Fernandez:2019:CCE

[3010] Francisco M. Fernández. Comment on: "On the computation of eigenvalues of the anharmonic Coulombic potential". *Journal of Mathematical*

Chemistry, 57(4):1181–1190, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01016-1`. See [2817].

Janani:2019:AEA

[3011] M. Janani, S. Devadharshini, and G. Hariharan. Analytical expressions of amperometric enzyme kinetics pertaining to the substrate concentration using wavelets. *Journal of Mathematical Chemistry*, 57(4): 1191–1200, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01017-0`.

Hsu:2019:NFS

[3012] Chieh-Wen Hsu, Chialiang Lin, Chenglian Liu, and T. E. Simos. A new four-stages two-step phase fitted scheme for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 57(4):1201–1229, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01018-z`.

Wang:2019:PPG

[3013] Yan Wang. The Pfaffian property of graphs on the Möbius strip based on topological resolution. *Journal of Mathematical Chemistry*, 57(4): 1230–1238, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01019-y`.

Verma:2019:CCM

[3014] Amit Kumar Verma and Sheerin Kayenat. Correction to: On the convergence of Mickens' type nonstandard finite difference schemes on Lane–Emden type equations. *Journal of Mathematical Chemistry*, 57(4):1239–1240, April 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01013-4; https://link.springer.com/content/pdf/10.1007/s10910-019-01013-4.pdf`. See [2880].

Vigo-Aguiar:2019:ICC

[3015] Jesus Vigo-Aguiar. International Conference on Computational and Mathematical Methods in Science and Engineering, held in Costa Ballena, Cádiz, Spain, July 9–13, 2018. *Journal of Mathematical Chemistry*, 57(5):1241–1242, May 2019. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01029-w; https://link.springer.com/content/pdf/10.1007/s10910-019-01029-w.pdf.

Recio:2019:CLL

[3016] Elena Recio, Tamara M. Garrido, Rafael de la Rosa, and María S. Bruzón. Conservation laws and Lie symmetries a $(2 + 1)$-dimensional thin film equation. *Journal of Mathematical Chemistry*, 57(5):1243–1251, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0945-y.

Gonzalez:2019:AFF

[3017] P. González, H. Idais, M. Pasadas, and M. Yasin. Approximation of fuzzy functions by fuzzy interpolating bicubic splines: 2018 CMMSE conference. *Journal of Mathematical Chemistry*, 57(5):1252–1267, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0946-x.

Argyros:2019:DMS

[3018] Ioannis K. Argyros, Á. A. Magreñán, L. Orcos, Íñigo Sarría, and Juan Antonio Sicilia. Different methods for solving STEM problems. *Journal of Mathematical Chemistry*, 57(5):1268–1281, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0950-1.

Chicharro:2019:SAI

[3019] Francisco I. Chicharro, Alicia Cordero, Neus Garrido, and Juan R. Torregrosa. Stability and applicability of iterative methods with memory. *Journal of Mathematical Chemistry*, 57(5):1282–1300, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0952-z.

Garrido:2019:SSC

[3020] T. M. Garrido, R. de la Rosa, E. Recio, and M. S. Bruzón. Symmetries, solutions and conservation laws for the $(2+1)$ filtration-absorption model. *Journal of Mathematical Chemistry*, 57(5):1301–1313, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-018-0955-9.

Urenda-Cazares:2019:NPU

[3021] E. Urenda-Cázares, P. B. Espinoza, A. Gallegos, R. Jaimes-Reátegui, J. E. Macías-Díaz, and H. Vargas-Rodríguez. The noisy Pais–

Uhlenbeck oscillator. *Journal of Mathematical Chemistry*, 57(5):1314–1329, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0966-6`.

Bayon:2019:IEP

[3022] L. Bayón, P. Fortuny Ayuso, J. A. Otero, P. M. Suárez, and C. Tasis. Influence of enzyme production dynamics on the optimal control of a linear unbranched chemical process. *Journal of Mathematical Chemistry*, 57(5):1330–1343, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0969-3`.

Amiri:2019:SAJ

[3023] A. R. Amiri, Alicia Cordero, M. T. Darvishi, and Juan R. Torregrosa. Stability analysis of Jacobian-free iterative methods for solving nonlinear systems by using families of m-th power divided differences. *Journal of Mathematical Chemistry*, 57(5):1344–1373, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0971-9`.

Ruiz:2019:PDM

[3024] Irene Luque Ruiz and Miguel Ángel Gómez-Nieto. Prediction of the datasets modelability for the building of QSAR classification models by means of the centroid based rivality index. *Journal of Mathematical Chemistry*, 57(5):1374–1393, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0972-8`.

Hendy:2019:EHN

[3025] Ahmed S. Hendy and Jorge E. Macías-Díaz. An efficient Hamiltonian numerical model for a fractional Klein–Gordon equation through weighted-shifted Grünwald differences. *Journal of Mathematical Chemistry*, 57 (5):1394–1412, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0973-7`.

Liu:2019:NEP

[3026] Shiwei Liu, Juan Zheng, and Yonglei Fang. A new embedded 4(3) pair of modified two-derivative Runge–Kutta methods with FSAL property for the numerical solution of the Schrödinger equation. *Journal of Mathematical Chemistry*, 57(5):1413–1426, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-0974-6`.

Pestana:2019:CGA

[3027] Domingo Pestana, José M. Sigarreta, and Eva Tourís. CMMSE 18: geometric-arithmetic index and line graph. *Journal of Mathematical Chemistry*, 57(5):1427–1447, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00993-z`.

Zafar:2019:GCF

[3028] Fiza Zafar, Alicia Cordero, Juan R. Torregrosa, and Aneeqa Rafi. A general class of four parametric with- and without memory iterative methods for nonlinear equations. *Journal of Mathematical Chemistry*, 57(5): 1448–1471, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00996-w`.

Martinez-Perez:2019:SRL

[3029] Álvaro Martínez-Pérez and José M. Rodríguez. Some results on lower bounds for topological indices. *Journal of Mathematical Chemistry*, 57 (5):1472–1495, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-018-00999-7`.

Yang:2019:TMV

[3030] Yanping Yang, Yonglei Fang, Kaimin Wang, and Xiong You. THDRK methods with vanished phase-lag and its first derivative for the Schrödinger equation. *Journal of Mathematical Chemistry*, 57(5):1496–1507, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01002-7`.

Argyros:2019:ELC

[3031] Ioannis K. Argyros, M. J. Legaz, Á. A. Magreñán, D. Moreno, and Juan Antonio Sicilia. Extended local convergence for some inexact methods with applications. *Journal of Mathematical Chemistry*, 57(5): 1508–1523, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01004-5`.

Rodriguez:2019:IID

[3032] José M. Rodríguez, José L. Sánchez, and José M. Sigarreta. Inequalities on the inverse degree index. *Journal of Mathematical Chemistry*, 57 (5):1524–1542, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01022-3.

Wu:2019:TFT

[3033] Ke Wu, Yonglei Fang, and Dewen Liu. Trigonometrically fitted two-step Obrechkoff linear methods for the Schrödinger equation. *Journal of Mathematical Chemistry*, 57(5):1543–1556, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01027-y.

Kumar:2019:RDD

[3034] Sunil Kumar, Joginder Singh, and Mukesh Kumar. A robust domain decomposition method for singularly perturbed parabolic reaction-diffusion systems. *Journal of Mathematical Chemistry*, 57(5):1557–1578, May 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01026-z.

Hulliger:2019:RTP

[3035] Jürg Hulliger and Rolf Hesterberg. Reversal transition for polar molecular crystals: critical clusters size analysis and Monte Carlo simulations. *Journal of Mathematical Chemistry*, 57(6):1579–1585, June 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01020-5.

Hou:2019:MLG

[3036] Yanzhen Hou, Antti J. Niemi, Xubiao Peng, and Nevena Ilieva. Myoglobin ligand gate mechanism analysis by a novel 3D visualization technique. *Journal of Mathematical Chemistry*, 57(6):1586–1597, June 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01021-4.

Medvedev:2019:TSM

[3037] Maxim A. Medvedev and T. E. Simos. A three-stages multistep teeming in phase algorithm for computational problems in chemistry. *Journal of Mathematical Chemistry*, 57(6):1598–1617, June 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01024-1.

Xu:2019:FAD

[3038] Kexiang Xu, Fang Gao, Kinkar Chandra Das, and Nenad Trinajstić. A formula with its applications on the difference of Zagreb in-

dices of graphs. *Journal of Mathematical Chemistry*, 57(6):1618–1626, June 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01025-0`.

Alolyan:2019:FSM

[3039] Ibraheem Alolyan and T. E. Simos. A four-stages multistep fraught in phase method for quantum chemistry problems. *Journal of Mathematical Chemistry*, 57(6):1627–1651, June 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01028-x`.

Luo:2019:MHH

[3040] Xiaopeng Luo, Xin Xu, and Herschel Rabitz. Meshless Hermite–HDMR finite difference method for high-dimensional Dirichlet problems. *Journal of Mathematical Chemistry*, 57(6):1652–1669, June 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01031-2`.

Lampart:2019:CBC

[3041] Marek Lampart and Tomás Martinovic. Chaotic behavior of the CML model with respect to the state and coupling parameters. *Journal of Mathematical Chemistry*, 57(6):1670–1681, June 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01023-2`.

Xu:2019:NMS

[3042] Xin Xu, Xiaopeng Luo, and Herschel Rabitz. Numerical meshless solution of high-dimensional sine-Gordon equations via Fourier HDMR–HC approximation. *Journal of Mathematical Chemistry*, 57(7):1683–1699, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01030-3`.

Fuster:2019:CAC

[3043] Robert Fuster, Maria T. Gassó, and Isabel Giménez. CMMSE algorithms for constructing doubly stochastic matrices with the relative gain array (combined matrix) $A \circ A^{-T}$. *Journal of Mathematical Chemistry*, 57(7):1700–1709, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01032-1`.

Xu:2019:MTS

[3044] Mingfei Xu and T. E. Simos. A multistage two-step fraught in phase scheme for problems in mathematical chemistry. *Journal of Mathematical Chemistry*, 57(7):1710–1731, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01033-0`.

Rai:2019:SLR

[3045] Prashant Rai, Khachik Sargsyan, Habib Najm, and So Hirata. Sparse low rank approximation of potential energy surfaces with applications in estimation of anharmonic zero point energies and frequencies. *Journal of Mathematical Chemistry*, 57(7):1732–1754, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01034-z`.

Miranda-Quintana:2019:IUS

[3046] Ramón Alain Miranda-Quintana, Taewon David Kim, Farnaz Heidar-Zadeh, and Paul W. Ayers. On the impossibility of unambiguously selecting the best model for fitting data. *Journal of Mathematical Chemistry*, 57(7):1755–1769, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01035-y`.

Tarko:2019:NCE

[3047] Laszlo Tarko. Novel criteria for elimination of the outliers in QSPR studies, when the 'forward stepwise' procedure is used. *Journal of Mathematical Chemistry*, 57(7):1770–1796, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01036-x`.

Dhatt:2019:EQS

[3048] Sharmistha Dhatt and Kinshuk Banerjee. Efficacy of quasi-steady-state approximation in Michaelis–Menten kinetics: a stochastic signature. *Journal of Mathematical Chemistry*, 57(7):1797–1805, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01038-9`.

Mukherjee:2019:SCM

[3049] Neetik Mukherjee and Amlan K. Roy. Some complexity measures in confined isotropic harmonic oscillator. *Journal of Mathematical Chemistry*, 57(7):1806–1821, August 2019. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01039-8.

Ceccato:2019:IOF

[3050] Alessandro Ceccato and Diego Frezzato. Inequalities for overdamped fluctuating systems. *Journal of Mathematical Chemistry*, 57(7):1822–1839, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01040-1.

Amore:2019:MRT

[3051] Paolo Amore and Francisco M. Fernández. On a model for rotational tunneling with a C_6-space-time symmetric analog. *Journal of Mathematical Chemistry*, 57(7):1840–1849, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01041-0.

Rosenfeld:2019:LFM

[3052] Vladimir R. Rosenfeld. Looking into the future of molecules with novel topological symmetries. *Journal of Mathematical Chemistry*, 57(7):1850–1867, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01042-z.

Arockiaraj:2019:TIS

[3053] Micheal Arockiaraj, Sandi Klavžar, Shagufa Mushtaq, and Krishnan Balasubramanian. Topological indices of the subdivision of a family of partial cubes and computation of SiO_2 related structures. *Journal of Mathematical Chemistry*, 57(7):1868–1883, August 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01043-y.

Balaji:2019:EOM

[3054] S. Balaji and G. Hariharan. An efficient operational matrix method for the numerical solutions of the fractional Bagley–Torvik equation using wavelets. *Journal of Mathematical Chemistry*, 57(8):1885–1901, September 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01047-8.

Macias-Diaz:2019:EFE

[3055] Jorge E. Macías-Díaz. An efficient and fully explicit model to simulate delayed activator-inhibitor systems with anomalous diffusion. *Journal*

of Mathematical Chemistry, 57(8):1902–1923, September 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01046-9`.

Dong:2019:ESS

[3056] Qian Dong, Ariadna J. Torres-Arenas, Guo-Hua Sun, O. Camacho-Nieto, Smain Femmam, and Shi-Hai Dong. Exact solutions of the sine hyperbolic type potential. *Journal of Mathematical Chemistry*, 57(8):1924–1931, September 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01045-w`.

He:2019:TSS

[3057] Ji-Huan He and Fei-Yu Ji. Taylor series solution for Lane–Emden equation. *Journal of Mathematical Chemistry*, 57(8):1932–1934, September 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01048-7`.

Somuncu:2019:CES

[3058] Elif Somuncu, Feda Oner, Metin Orbay, and Bahtiyar A. Mamedov. A comparative evaluation of speed of sound and specific heat capacities of gases by using the quantum mechanical and classical second virial coefficients. *Journal of Mathematical Chemistry*, 57(8):1935–1948, September 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01049-6`.

Wang:2019:QED

[3059] Hongxia Wang, Qingyuan Xia, and Hui Liu. Quick estimation of $f(E)$ in the distributed activation energy model (DAEM): an inverse problem approach. *Journal of Mathematical Chemistry*, 57(8):1949–1972, September 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01044-x`.

Laurinavicius:2019:DDM

[3060] Valdas Laurinavičius, Feliksas Ivanauskas, and Anatolij Nečiporenko. Drug delivery mathematical modeling for pressure controlled bioreactor. *Journal of Mathematical Chemistry*, 57(8):1973–1982, September 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01050-z`.

Lv:2019:RKT

[3061] Jieyin Lv and T. E. Simos. A Runge–Kutta type crowded in phase algorithm for quantum chemistry problems. *Journal of Mathematical Chemistry*, 57(8):1983–2006, September 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01051-y`.

Jia:2019:SPM

[3062] Ji-Teng Jia. On a structure-preserving matrix factorization for the determinants of cyclic pentadiagonal Toeplitz matrices. *Journal of Mathematical Chemistry*, 57(8):2007–2017, September 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01053-w`.

Qiu:2019:PPF

[3063] Junlai Qiu, Junjie Huang, and T. E. Simos. A perfect in phase FD algorithm for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 57(9):2019–2048, October 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01061-w`.

Zhang:2019:MSA

[3064] Xunying Zhang and T. E. Simos. A multiple stage absolute in phase scheme for chemistry problems. *Journal of Mathematical Chemistry*, 57(9):2049–2074, October 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01054-9`.

He:2019:VPT

[3065] Ji-Huan He and Chang Sun. A variational principle for a thin film equation. *Journal of Mathematical Chemistry*, 57(9):2075–2081, October 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01063-8`.

Belkic:2019:ASC

[3066] Dzevad Belkić and Karen Belkić. Automatic self-correcting in signal processing for magnetic resonance spectroscopy: noise reduction, resolution improvement and splitting overlapped peaks. *Journal of Mathematical Chemistry*, 57(9):2082–2109, October 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01060-x; https://link.springer.com/content/pdf/10.1007/s10910-019-01060-x.pdf`.

Li:2019:MDO

[3067] Genyuan Li. Molecular discovery by optimal sequential search. *Journal of Mathematical Chemistry*, 57(9):2110–2141, October 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01062-9`.

Tandon:2019:NSA

[3068] Hiteshi Tandon, Tanmoy Chakraborty, and Vandana Suhag. A new scale of atomic static dipole polarizability invoking other periodic descriptors. *Journal of Mathematical Chemistry*, 57(9):2142–2153, October 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01055-8`.

Wu:2019:ITF

[3069] Re-Bing Wu, Qiuyang Sun, Tak san Ho, and Herschel Rabitz. Inherently trap-free convex landscapes for fully quantum optimal control. *Journal of Mathematical Chemistry*, 57(9):2154–2167, October 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01059-4`.

Tokmachev:2019:SCD

[3070] M. G. Tokmachev and N. A. Tikhonov. Simulation of capacitive deionization accounting the change of Stern layer thickness. *Journal of Mathematical Chemistry*, 57(10):2169–2181, November 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01064-7`.

Carbo-Dorca:2019:HDA

[3071] Ramon Carbó-Dorca and Tanmoy Chakraborty. Hypercubes defined on n-ary sets, the Erdős–Faber–Lovász conjecture on graph coloring, and the description spaces of polypeptides and RNA. *Journal of Mathematical Chemistry*, 57(10):2182–2194, November 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01065-6`.

Grifall-Sabo:2019:KME

[3072] John C. Grifall-Sabo, Trenner Nolan, Matthew M. Beck, and Christopher J. Barile. Kinetic modeling of electrocatalytic oxygen reduction products from lipid-modified electrodes. *Journal of Mathematical Chemistry*, 57(10):2195–2207, November 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01066-5`.

Medvedeva:2019:APF

[3073] Marina A. Medvedeva and T. E. Simos. An accomplished phase FD process for DEs in chemistry. *Journal of Mathematical Chemistry*, 57(10): 2208–2228, November 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01067-4`.

Padilha:2019:SLJ

[3074] F. R. R. Padilha and A. L. De Bortoli. Solutions for a laminar jet diffusion flame of methyl formate using a skeletal mechanism obtained by applying ANNs. *Journal of Mathematical Chemistry*, 57(10):2229–2247, November 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01068-3`.

Chen:2019:TPA

[3075] Hanlin Chen and Qiuzhi Guo. Tutte polynomials of alternating polycyclic chains. *Journal of Mathematical Chemistry*, 57(10):2248–2260, November 2019. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01069-2`.

Carbo-Dorca:2020:CLT

[3076] Ramon Carbó-Dorca. Cantor-like transfinite sequences and Gödel-like incompleteness revealed by means of Mersenne transfinite dimensional boolean hypercube concatenation. *Journal of Mathematical Chemistry*, 58(1):1–5, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01075-4`.

Ma:2020:IPF

[3077] Yu-Yu Ma, Chia-Liang Lin, and T. E. Simos. An integrated in phase FD procedure for DiffEqns in chemical problems. *Journal of Mathematical Chemistry*, 58(1):6–28, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01070-9`.

Lemus:2020:AAC

[3078] Renato Lemus. An algebraic approach to calculate Franck–Condon factors. *Journal of Mathematical Chemistry*, 58(1):29–55, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01071-8`.

Hernandez:2020:CAM

[3079] Bryan S. Hernandez, Eduardo R. Mendoza, and Aurelio A. de los Reyes V. A computational approach to multistationarity of power-law kinetic systems. *Journal of Mathematical Chemistry*, 58(1):56–87, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01072-7`.

Marmorino:2020:ULB

[3080] M. G. Marmorino. Upper and lower bounds to atomic radial position moments. *Journal of Mathematical Chemistry*, 58(1):88–113, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01073-6`.

Tsitouras:2020:EOP

[3081] Ch. Tsitouras. Eighth order, phase-fitted, six-step methods for solving $y'' = f(x, y)$. *Journal of Mathematical Chemistry*, 58(1):114–125, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01074-5`.

Ghosh:2020:IDE

[3082] P. Ghosh and J. F. Peters. Impulsive differential equation model in methanol poisoning detoxification. *Journal of Mathematical Chemistry*, 58(1):126–145, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01076-3`.

Belkic:2020:FSA

[3083] Dzevad Belkić and Karen Belkić. Feasibility study for applying the lower-order derivative fast Padé transform to measured time signals. *Journal of Mathematical Chemistry*, 58(1):146–177, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01077-2; https://link.springer.com/content/pdf/10.1007/s10910-019-01077-2.pdf`.

Konguetsof:2020:ADF

[3084] A. Konguetsof. Algorithm for the development of families of numerical methods based on phase-lag Taylor series. *Journal of Mathematical Chemistry*, 58(1):178–203, January 2020. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01078-1.

Balasubramanian:2020:CCH

[3085] Krishnan Balasubramanian. Computational combinatorics of hyperplane colorings of 6D-hypercube for all irreducible representations and applications. *Journal of Mathematical Chemistry*, 58(1):204–272, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01079-0.

Bayon:2020:ILP

[3086] L. Bayón, P. Fortuny Ayuso, J. M. Grau, M. M. Ruiz, and P. M. Suárez. Irreversible linear pathways in enzymatic reactions: analytical solution using the homotopy perturbation method. *Journal of Mathematical Chemistry*, 58(1):273–291, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01080-7.

Krajnak:2020:PSS

[3087] Vladimír Krajnák and Holger Waalkens. Phase space structures causing the reaction rate decrease in the collinear hydrogen exchange reaction. *Journal of Mathematical Chemistry*, 58(1):292–339, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01083-4; https://link.springer.com/content/pdf/10.1007/s10910-019-01083-4.pdf.

Mihalka:2020:VPN

[3088] Zsuzsanna É. Mihálka, Ádám Margócsy, Ágnes Szabados, and Péter R. Surján. On the variational principle for the non-linear Schrödinger equation. *Journal of Mathematical Chemistry*, 58(1):340–351, January 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01082-5; https://link.springer.com/content/pdf/10.1007/s10910-019-01082-5.pdf.

Hao:2020:PFF

[3089] Sheng Hao and T. E. Simos. A phase fitted FinDiff process for DifEquns in quantum chemistry. *Journal of Mathematical Chemistry*, 58(2):353–381, February 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01081-6.

Putthikorn:2020:EBD

[3090] Sasipim Putthikorn, Pornrat Ruengrot, and Duangkamon Baowan. Energy behaviour of Doxorubicin interacting with peptide nanotubes. *Journal of Mathematical Chemistry*, 58(2):382–392, February 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01087-0`.

Hua:2020:ISB

[3091] Wei Hua, Shi Xing Liu, and Teng Zhang. Interferences and solitons in the Bose–Einstein condensates with two- and three-body interactions. *Journal of Mathematical Chemistry*, 58(2):393–406, February 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01093-2`.

Tong:2020:CPF

[3092] Xing Tong and T. E. Simos. A complete in phase FinitDiff procedure for DiffEquns in chemistry. *Journal of Mathematical Chemistry*, 58(2): 407–438, February 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01095-0`.

Rodriguez-Velazquez:2020:CRP

[3093] Juan A. Rodríguez-Velázquez and Alexandru T. Balaban. Criteria for ranking (poly)cyclic chemical constitutional graphs and their vertices via centrality measures. *Journal of Mathematical Chemistry*, 58(2): 439–457, February 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01096-z`.

Balasubramanian:2020:ERS

[3094] Krishnan Balasubramanian. Enumeration of relativistic states for superheavy and transactinide dimers in the periodic table. *Journal of Mathematical Chemistry*, 58(2):458–496, February 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01098-x`.

Valenzuela:2020:HBB

[3095] Luis Miguel Valenzuela, Gamaliel Blé, Manuel Falconi, and David Guerrero. Hopf and Bautin bifurcations in a generalized Lengyel–Epstein system. *Journal of Mathematical Chemistry*, 58(2):497–515, February 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01099-w`.

Doktorov:2020:TIE

[3096] Alexander B. Doktorov and Alexander A. Kipriyanov. Theoretical investigation of exciplex generation under X-ray irradiation of non-polar solutions. *Journal of Mathematical Chemistry*, 58(2):516–542, February 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01100-x`.

Vigo-Aguiar:2020:GEF

[3097] Jesús Vigo-Aguiar. Guest Editor foreword for CMMSE special issue of *Journal of Mathematical Chemistry*. *Journal of Mathematical Chemistry*, 58(3):543, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01106-5; https://link.springer.com/content/pdf/10.1007/s10910-020-01106-5.pdf`.

Urenda-Cazares:2020:MMC

[3098] E. Urenda-Cázares, A. Gallegos, and J. E. Macías-Díaz. A mathematical model that combines chemotherapy and oncolytic virotherapy as an alternative treatment against a glioma. *Journal of Mathematical Chemistry*, 58(3):544–554, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01084-3`.

Chicharro:2020:CMBa

[3099] Francisco I. Chicharro, Alicia Cordero, Tobías H. Martínez, and Juan R. Torregrosa. CMMSE-2019 mean-based iterative methods for solving nonlinear chemistry problems. *Journal of Mathematical Chemistry*, 58(3):555–572, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01085-2`. See [3100].

Chicharro:2020:CMBb

[3100] Francisco I. Chicharro, Alicia Cordero, Tobías H. Martínez, and Juan R. Torregrosa. Correction to: Mean-based iterative methods for solving nonlinear chemistry problems. *Journal of Mathematical Chemistry*, 58(3):573, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01090-5; https://link.springer.com/content/pdf/10.1007/s10910-019-01090-5.pdf`. See [3099].

Rao:2020:DSW

[3101] S. Chandra Sekhara Rao, Sunil Kumar, and Joginder Singh. A discrete Schwarz waveform relaxation method of higher order for singularly perturbed parabolic reaction-diffusion problems. *Journal of Mathematical Chemistry*, 58(3):574–594, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01086-1`.

Trapeznikova:2020:CEA

[3102] Marina Trapeznikova, Natalia Churbanova, and Anastasia Lyupa. CMMSE 2019: an explicit algorithm for the simulation of non-isothermal multiphase multicomponent flow in a porous medium. *Journal of Mathematical Chemistry*, 58(3):595–611, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01088-z`.

Datsko:2020:MMP

[3103] B. Datsko, M. Kutniv, and A. Włoch. Mathematical modelling of pattern formation in activator-inhibitor reaction-diffusion systems with anomalous diffusion. *Journal of Mathematical Chemistry*, 58(3):612–631, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01089-y`.

Carballosa:2020:RBS

[3104] Walter Carballosa, Ana Granados, Domingo Pestana, Ana Portilla, and José M. Sigarreta. Relations between some topological indices and the line graph. *Journal of Mathematical Chemistry*, 58(3):632–646, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01091-4`.

Akhrif:2020:AGO

[3105] R. Akhrif, A. Kouibia, and M. Pasadas. Approximation of generalized offset surfaces by bicubic splines. *Journal of Mathematical Chemistry*, 58 (3):647–662, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01092-3`.

Aarthika:2020:NUD

[3106] K. Aarthika, V. Shanthi, and Higinio Ramos. A non-uniform difference scheme for solving singularly perturbed 1D-parabolic reaction-

convection-diffusion systems with two small parameters and discontinuous source terms. *Journal of Mathematical Chemistry*, 58(3):663–685, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01094-1`.

Maroju:2020:LCF

[3107] P. Maroju, Á. A. Magreñán, Í. Sarría, and Abhimanyu Kumar. Local convergence of fourth and fifth order parametric family of iterative methods in Banach spaces. *Journal of Mathematical Chemistry*, 58(3): 686–705, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01097-y`.

Argyros:2020:WCI

[3108] Ioannis K. Argyros, Á. Alberto Magreñán, Daniel Moreno, Lara Orcos, and Juan Antonio Sicilia. Weaker conditions for inexact mutitpoint Newton-like methods. *Journal of Mathematical Chemistry*, 58(3): 706–716, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01101-w`.

Liu:2020:OTS

[3109] Shiwei Liu, Juan Zheng, and Yonglei Fang. Obrechkoff two-step method fitted with Fourier spectrum for undamped Duffing equation. *Journal of Mathematical Chemistry*, 58(3):717–734, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01102-9`.

Macias-Diaz:2020:SCI

[3110] Jorge E. Macías-Díaz and Ahmed S. Hendy. On the stability and convergence of an implicit logarithmic scheme for diffusion equations with nonlinear reaction. *Journal of Mathematical Chemistry*, 58(3): 735–749, March 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01103-8`.

Cordero:2020:SVH

[3111] Alicia Cordero, Higinio Ramos, and Juan R. Torregrosa. Some variants of Halley's method with memory and their applications for solving several chemical problems. *Journal of Mathematical Chemistry*, 58 (4):751–774, April 2020. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01108-3.

Saez:2020:LSC

[3112] S. Sáez, R. de la Rosa, E. Recio, T. M. Garrido, and M. S. Bruzón. Lie symmetries and conservation laws for a generalized $(2 + 1)$-dimensional nonlinear evolution equation. *Journal of Mathematical Chemistry*, 58 (4):775–798, April 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01111-8.

Khammahawong:2020:CSA

[3113] K. Khammahawong, P. Kumam, and P. Chaipunya. On the convergence of splitting algorithm for mixed equilibrium problems on Hadamard manifolds. *Journal of Mathematical Chemistry*, 58(4):799–815, April 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01121-6.

Argyros:2020:NTS

[3114] I. K. Argyros, Á. A. Magreñán, D. F. Yáñez, and J. A. Sicilia. A new technique for studying the convergence of Newton's solver with real life applications. *Journal of Mathematical Chemistry*, 58(4):816–830, April 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01119-0.

Bruzon:2020:PSB

[3115] M. S. Bruzón, A. P. Márquez, E. Recio, T. M. Garrido, and R. de la Rosa. Potential systems of a Buckley–Leverett equation: Lie point symmetries and conservation laws. *Journal of Mathematical Chemistry*, 58 (4):831–840, April 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01110-9.

Alshomrani:2020:LCP

[3116] Ali Saleh Alshomrani, Ramandeep Behl, and P. Maroju. Local convergence of parameter based method with six and eighth order of convergence. *Journal of Mathematical Chemistry*, 58(4):841–853, April 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01113-6.

Behl:2020:GCO

[3117] Ramandeep Behl, Ali Saleh Alshomrani, and Changbum Chun. A general class of optimal eighth-order derivative free methods for nonlinear equations. *Journal of Mathematical Chemistry*, 58(4):854–867, April 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01115-4`.

Behl:2020:EFC

[3118] Ramandeep Behl. An efficient family of Chebyshev–Halley's methods for system of nonlinear equations. *Journal of Mathematical Chemistry*, 58 (4):868–885, April 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01114-5`.

Raychaudhury:2020:UGV

[3119] Chandan Raychaudhury and Debnath Pal. Usefulness of graph vertex complexity and class partial information content in explaining gas phase thermal entropy of chemical compounds. *Journal of Mathematical Chemistry*, 58(5):887–892, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01118-1`.

Antuna:2020:SWK

[3120] Almudena Antuña, Juan L. G. Guirao, and Miguel A. López. Shannon–Whittaker–Kotel'nikov's theorem generalized revisited. *Journal of Mathematical Chemistry*, 58(5):893–905, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01037-w`.

Wang:2020:EWC

[3121] Li Wang, Junpeng Kang, Jiping Xu, Huiyan Zhang, Xiaoyi Wang, Jiabin Yu, Qian Sun, and Zhiyao Zao. Early warning of cyanobacteria blooms outbreak based on stoichiometric analysis and catastrophe theory model. *Journal of Mathematical Chemistry*, 58(5):906–921, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-019-01052-x`.

Elgendy:2020:ESA

[3122] Abd Elfattah T. Elgendy, Abdel-Haleem Abdel-Aty, Amr A. Youssef, Moaiad A. A. Khder, Khaled Lotfy, and Saud Owyed. Exact solution of Arrhenius equation for non-isothermal kinetics at constant heating rate and n-th order of reaction. *Journal of Mathematical Chemistry*, 58

(5):922–938, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01056-7.

Alkhateeb:2020:SFN

[3123] Sadah A. Alkhateeb and S. Abdel-Khalek. Some features of the nonlocal correlation and geometric phase of the quantum system in two-mode nondegenerate entangled states. *Journal of Mathematical Chemistry*, 58 (5):939–949, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01057-6.

Algarni:2020:TCR

[3124] Ali Algarni, Abdullah M. Almarashi, G. A. Abd-Elmougod, and Z. A. Abo-Eleneen. Two compound Rayleigh lifetime distributions in analyses the jointly type-II censoring samples: DSGT2018. *Journal of Mathematical Chemistry*, 58(5):950–966, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-019-01058-5.

Roul:2020:SOO

[3125] Pradip Roul and V. M. K. Prasad Goura. A sixth order optimal B-spline collocation method for solving Bratu's problem. *Journal of Mathematical Chemistry*, 58(5):967–988, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01105-6.

Edet:2020:TPD

[3126] C. O. Edet, U. S. Okorie, G. Osobonye, A. N. Ikot, G. J. Rampho, and R. Sever. Thermal properties of Deng–Fan–Eckart potential model using Poisson summation approach. *Journal of Mathematical Chemistry*, 58 (5):989–1013, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01107-4.

Klein:2020:TSG

[3127] D. J. Klein, T. Goswami, and Y. P. Ortiz. Translationally symmetric graphene strips. *Journal of Mathematical Chemistry*, 58(5): 1014–1024, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01112-7.

Tandon:2020:CAR

[3128] Hiteshi Tandon, Prabhat Ranjan, Tanmoy Chakraborty, and Vandana Suhag. Computation of absolute radii of 103 elements of the periodic table in terms of nucleophilicity index. *Journal of Mathematical Chemistry*, 58(5):1025–1040, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01117-2`.

Alici:2020:GSS

[3129] H. Alici and T. Tanriverdi. General solution of the Schrödinger equation for some trigonometric potentials. *Journal of Mathematical Chemistry*, 58(5):1041–1057, May 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01120-7`.

Chen:2020:PFF

[3130] Xiaoping Chen and T. E. Simos. A phase fitted FiniteDiffr process for DiffrntEqutns in chemistry. *Journal of Mathematical Chemistry*, 58(6): 1059–1090, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01104-7`.

Lin:2020:CPF

[3131] Chia-Liang Lin and T. E. Simos. A complete in phase FiniteDiffrnc algorithm for DiffrntEqutins in chemistry. *Journal of Mathematical Chemistry*, 58(6):1091–1132, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01116-3`.

Belkic:2020:TCS

[3132] Dzevad Belkić. Total cross sections in five methods for two-electron capture by alpha particles from helium: CDW-4B, BDW-4B, BCIS-4B, CDW–EIS-4B and CB1-4B. *Journal of Mathematical Chemistry*, 58(6):1133–1176, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01123-4; https://link.springer.com/content/pdf/10.1007/s10910-020-01123-4.pdf`.

Xavier:2020:IPP

[3133] Antony Xavier, Santiagu Theresal, and S. Maria Jesu Raja. Induced H-packing k-partition number for certain nanotubes and chemical graphs. *Journal of Mathematical Chemistry*, 58(6):1177–1196,

June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01124-3.

Zhao:2020:FPF

[3134] Zhen Zhao, Jun Luo, Chia-Liang Lin, and T. E. Simos. Full in phase finite difference algorithm for differential equations in quantum chemistry. *Journal of Mathematical Chemistry*, 58(6):1197–1218, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01125-2.

Gromov:2020:AFT

[3135] Dmitry Gromov and Alexander Toikka. On an alternative formulation of the thermodynamic stability condition. *Journal of Mathematical Chemistry*, 58(6):1219–1229, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01126-1.

Saranya:2020:SSC

[3136] K. Saranya, V. Mohan, and L. Rajendran. Steady-state concentrations of carbon dioxide absorbed into phenyl glycidyl ether solutions by residual method. *Journal of Mathematical Chemistry*, 58(6):1230–1246, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01127-0.

Farantos:2020:HTE

[3137] Stavros C. Farantos. Hamiltonian thermodynamics in the extended phase space: a unifying theory for non-linear molecular dynamics and classical thermodynamics. *Journal of Mathematical Chemistry*, 58(6):1247–1280, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01128-z.

Shults:2020:MCM

[3138] O. V. Shults. Method for calculating material balance of complex process flowcharts. *Journal of Mathematical Chemistry*, 58(6):1281–1290, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01129-y.

Sayevand:2020:FEH

[3139] K. Sayevand. On a flexible extended homotopy perturbation method and its applications in applied chemistry. *Journal of Mathematical Chemistry*, 58(6):1291–1305, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01130-5`.

Li:2020:NCC

[3140] Risong Li and Yu Zhao. Note on chaos of a coupled lattice system related with the Belusov–Zhabotinskii reaction. *Journal of Mathematical Chemistry*, 58(6):1306–1311, June 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01122-5`.

Luo:2020:PFM

[3141] Jun Luo, Zhen Zhao, Chia-Liang Lin, and T. E. Simos. Phase fitted method for quantum chemistry problems. *Journal of Mathematical Chemistry*, 58(7):1313–1336, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01131-4`.

Chang:2020:FHT

[3142] Jing Chang and Ramon Carbó-Dorca. Fuzzy hypercubes and their time-like evolution. *Journal of Mathematical Chemistry*, 58(7):1337–1344, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01137-y`.

Gao:2020:NGT

[3143] Wei Gao, Juan Luis García Guirao, and Hualong Wu. Nordhaus–Gaddum type inequalities for some distance-based indices of bipartite molecular graphs. *Journal of Mathematical Chemistry*, 58(7):1345–1352, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01139-w`.

Vigdorowitsch:2020:PAF

[3144] Michael V. Vigdorowitsch, Liudmila E. Tsygankova, and Vyacheslav D. Prokhorenkov. The polylogarithmic adsorption function: a linear energetic surface heterogeneity. *Journal of Mathematical Chemistry*, 58(7):1353–1363, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01133-2`.

Fujita:2020:SIE

[3145] Shinsaku Fujita. Symmtry-itemized enumeration of compounds derived from different $\vec{I}_h$-skeletons by means of combined-permutation representations and newly-developed GAP functions. *Journal of Mathematical Chemistry*, 58(7):1364–1408, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01132-3`.

Morales-Bayuelo:2020:MQS

[3146] Alejandro Morales-Bayuelo, José Catalán, Leonor Alvarado-Soto, and Rodrigo Ramírez-Tagle. Molecular quantum similarity studies and molecular properties of the tungsten intermediates $[W_6I_{14}]^{2-}$ clusters. *Journal of Mathematical Chemistry*, 58(7):1409–1419, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01141-2`.

Orpel:2020:EPS

[3147] Aleksandra Orpel. Existence and properties of solutions for boundary value problems based on the nonlinear reactor dynamics. *Journal of Mathematical Chemistry*, 58(7):1420–1436, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01134-1; https://link.springer.com/content/pdf/10.1007/s10910-020-01134-1.pdf`.

Deng:2020:ECB

[3148] Kecai Deng and Shuchao Li. Extremal catacondensed benzenoids with respect to the Mostar index. *Journal of Mathematical Chemistry*, 58(7):1437–1465, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01135-0`.

Jia:2020:GSM

[3149] Ji-Teng Jia and Tomohiro Sogabe. Generalized Sherman–Morrison–Woodbury formula based algorithm for the inverses of opposite-bordered tridiagonal matrices. *Journal of Mathematical Chemistry*, 58(7):1466–1480, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01138-x`.

Qin:2020:KSM

[3150] Yupeng Qin, Qingjun Lou, Zhen Wang, and Li Zou. Kudryashov and Sinelshchikov's method for solving the radial oscillation problem of multielectron bubbles in liquid helium. *Journal of Mathematical Chemistry*, 58(7):1481–1488, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01145-y`.

Marquez:2020:CLS

[3151] Almudena del Pilar Márquez and María de los Santos Bruzón. Conservation laws and symmetry analysis for a quasi-linear strongly-damped wave equation. *Journal of Mathematical Chemistry*, 58(7):1489–1498, August 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01146-x`.

Medvedeva:2020:PFA

[3152] Marina A. Medvedeva and T. E. Simos. Phase fitted algorithm for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 58(8):1499–1530, September 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01142-1`.

Skakauskas:2020:MT

[3153] V. Skakauskas and P. Katauskis. Modelling of the "surface explosion" of the NO + H_2 reaction over supported catalysts. *Journal of Mathematical Chemistry*, 58(8):1531–1547, September 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01149-8`.

Smith:2020:PSG

[3154] William R. Smith. A precise, simple and general Basic Le Châtelier Principle based on elementary calculus: What Le Châtelier had in mind? *Journal of Mathematical Chemistry*, 58(8):1548–1570, September 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01140-3`.

Cinal:2020:HAN

[3155] M. Cinal. Highly accurate numerical solution of Hartree–Fock equation with pseudospectral method for closed-shell atoms. *Journal of Mathematical Chemistry*, 58(8):1571–1600, September 2020. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01144-z.

Roul:2020:BCM

[3156] Pradip Roul and V. M. K. Prasad Goura. A Bessel collocation method for solving Bratu's problem. *Journal of Mathematical Chemistry*, 58(8): 1601–1614, September 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01147-w.

Din:2020:DBA

[3157] Qamar Din and Kamran Haider. Discretization, bifurcation analysis and chaos control for Schnakenberg model. *Journal of Mathematical Chemistry*, 58(8):1615–1649, September 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01154-x.

Sarapat:2020:MCN

[3158] Pakhapoom Sarapat, Ngamta Thamwattana, and Duangkamon Baowan. Modelling carbon nanocones for selective filter. *Journal of Mathematical Chemistry*, 58(8):1650–1662, September 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01153-y.

Lin:2020:ESS

[3159] Bin Lin. An efficient spline scheme of the coupled nonlinear Schrödinger equations. *Journal of Mathematical Chemistry*, 58(8):1663–1679, September 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01143-0.

Wang:2020:FDM

[3160] Zenggui Wang and T. E. Simos. A finite difference method with zero phase-lag and its derivatives for quantum chemistry problems. *Journal of Mathematical Chemistry*, 58(8):1680–1710, September 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01150-1.

Adams:2020:KTP

[3161] Colin Adams, Judah Devadoss, and Alireza Mashaghi. Knot theory for proteins: Gauss codes, quandles and bondles. *Journal of Mathematical Chemistry*, 58(8):1711–1736, September 2020. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01151-0.

Thiruvengadam:2020:GMU

[3162] Sudharsan Thiruvengadam, Matthew Murphy, and Karol Miller. A generalised methodology using conformal geometric algebra for mathematical chemistry. *Journal of Mathematical Chemistry*, 58(8):1737–1783, September 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01155-w.

Lin:2020:CPM

[3163] Chia-Liang Lin and T. E. Simos. Complete in phase method for problems in chemistry. *Journal of Mathematical Chemistry*, 58(9):1785–1814, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01136-z.

Chang:2020:QSD

[3164] Jing Chang and Ramon Carbó-Dorca. A quantum similarity discussion about Einstein–Podolsky–Rosen (EPR) paradox in Gaussian enfolded spaces. *Journal of Mathematical Chemistry*, 58(9):1815–1827, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01158-7.

Jia:2020:NAD

[3165] Ji-Teng Jia. Numerical algorithms for the determinants of opposite-bordered and singly-bordered tridiagonal matrices. *Journal of Mathematical Chemistry*, 58(9):1828–1845, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01157-8.

Li:2020:TPR

[3166] Qishun Li, Shuchao Li, and Leilei Zhang. Two-point resistances in the generalized phenylenes. *Journal of Mathematical Chemistry*, 58(9):1846–1873, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01152-z.

Singh:2020:ITS

[3167] Randhir Singh. An iterative technique for solving a class of local and nonlocal elliptic boundary value problems. *Journal of Mathematical Chem-*

istry, 58(9):1874–1894, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01159-6`.

Anderson:2020:CRN

[3168] David F. Anderson, James D. Brunner, and Matthew D. Johnston. On classes of reaction networks and their associated polynomial dynamical systems. *Journal of Mathematical Chemistry*, 58(9):1895–1925, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01148-9`.

Thiruvengadam:2020:CAB

[3169] Sudharsan Thiruvengadam, Matthew Murphy, and Karol Miller. A Clifford Algebra-based mathematical model for the determination of critical temperatures in superconductors. *Journal of Mathematical Chemistry*, 58(9):1926–1986, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01156-9`.

Khalsaraei:2020:NCM

[3170] Mohammad Mehdizadeh Khalsaraei, Ali Shokri, and Maryam Molayi. The new class of multistep multiderivative hybrid methods for the numerical solution of chemical stiff systems of first order IVPs. *Journal of Mathematical Chemistry*, 58(9):1987–2012, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01160-z`.

Guerrero-Sanchez:2020:CEB

[3171] Y. Guerrero-Sánchez, M. Fernández-Martínez, and F. J. Gómez-García. Chemical effect of bisphosphonates on the bone trabeculate of jaws via fractal dimension. *Journal of Mathematical Chemistry*, 58(9):2013–2023, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01163-w`.

Medvedev:2020:FDM

[3172] Maxim A. Medvedev and T. E. Simos. A finite difference method with phase-lag and its derivatives equal to zero for problems in chemistry. *Journal of Mathematical Chemistry*, 58(9):2024–2060, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01161-y`.

Adamer:2020:FTC

[3173] Michael F. Adamer and Martin Helmer. Families of toric chemical reaction networks. *Journal of Mathematical Chemistry*, 58(9):2061–2093, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01162-x`.

Fernandez:2020:ATN

[3174] Francisco M. Fernández. Algebraic treatment of non-Hermitian quadratic Hamiltonians. *Journal of Mathematical Chemistry*, 58(9):2094–2107, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01165-8`.

Li:2020:SPI

[3175] Fengwei Li, Xueliang Li, and Hajo Broersma. Spectral properties of inverse sum indeg index of graphs. *Journal of Mathematical Chemistry*, 58(9):2108–2139, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01170-x`.

Murugan:2020:TTB

[3176] Rajamanickam Murugan. Theory of transcription bursting: stochasticity in the transcription rates. *Journal of Mathematical Chemistry*, 58(9):2140–2187, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01166-7`.

Tandon:2020:FAC

[3177] Hiteshi Tandon, Tanmoy Chakraborty, and Vandana Suhag. A fundamental approach to compute atomic electrophilicity index. *Journal of Mathematical Chemistry*, 58(9):2188–2196, October 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01176-5`.

Dong:2020:SES

[3178] Qian Dong, Guo-Hua Sun, and Shi-Hai Dong. Semi-exact solutions of sextic potential plus a centrifugal term. *Journal of Mathematical Chemistry*, 58(10):2197–2203, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01169-4`. See comment [3447].

Doslic:2020:NPO

[3179] Tomislav Doslić. Nice pairs of odd cycles in fullerene graphs. *Journal of Mathematical Chemistry*, 58(10):2204–2222, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01171-w`.

Doslic:2020:PSF

[3180] Tomislav Doslić, Meysam Taheri-Dehkordi, and Gholam Hossein Fath-Tabar. Packing stars in fullerenes. *Journal of Mathematical Chemistry*, 58(10):2223–2244, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01177-4`.

He:2020:HPM

[3181] Ji-Huan He and Yusry O. El-Dib. Homotopy perturbation method for Fangzhu oscillator. *Journal of Mathematical Chemistry*, 58(10):2245–2253, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01167-6`.

Dede:2020:ESS

[3182] Yavuz Dede, Soydan Yalcin, and Muhammed Buyuktemiz. Excited state structures projected onto two dimensions: correlations with luminescent behavior. *Journal of Mathematical Chemistry*, 58(10):2254–2272, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01175-6`.

Carballosa:2020:RBG

[3183] Walter Carballosa, Domingo Pestana, and Eva Tourís. Relations between the general sum connectivity index and the line graph. *Journal of Mathematical Chemistry*, 58(10):2273–2290, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01180-9`.

Awasthi:2020:NUP

[3184] Anjali Awasthi, Vikash Verma, and Aashees Awasthi. Nonlinear ultrasound propagation in formamide + 2-methoxyethanol/2-ethoxyethanol solvent systems at temperatures ranging from 303.15 to 323.15 K. *Journal of Mathematical Chemistry*, 58(10):2291–2312, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01181-8`.

Archibald:2020:FHW

[3185] M. Archibald, S. Currie, and M. Nowaczyk. Finding the hole in a wall. *Journal of Mathematical Chemistry*, 58(10):2313–2323, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01178-3`.

Medvedev:2020:NFS

[3186] Maxim A. Medvedev and T. E. Simos. New FD scheme with vanished phase-lag and its derivatives up to order six for problems in chemistry. *Journal of Mathematical Chemistry*, 58(10):2324–2360, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01168-5`.

Wang:2020:NAE

[3187] Zenggui Wang and T. E. Simos. A new algorithm with eliminated phase-lag and its derivatives up to order five for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 58(10):2361–2398, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01164-9`.

Popov:2020:CLS

[3188] A. Popov and V. Popov. Calculation of lattice sums of general type. *Journal of Mathematical Chemistry*, 58(10):2399–2414, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01182-7`.

Saez:2020:SAG

[3189] S. Sáez. Symmetry analysis of a generalized 2D Zakharov–kuznetsov-Burgers equation with a variable dissipation. *Journal of Mathematical Chemistry*, 58(10):2415–2424, November 2020. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01185-4`.

Paldus:2021:MEUa

[3190] Josef Paldus. Matrix elements of unitary group generators in many-fermion correlation problem. I. tensorial approaches. *Journal of Mathematical Chemistry*, 59(1):1–36, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01172-9`.

Paldus:2021:MEUb

[3191] Josef Paldus. Matrix elements of unitary group generators in many-fermion correlation problem. II. Graphical methods of spin algebras. *Journal of Mathematical Chemistry*, 59(1):37–71, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01173-8`.

Paldus:2021:MEUc

[3192] Josef Paldus. Matrix elements of unitary group generators in many-fermion correlation problem. III. Green–Gould approach. *Journal of Mathematical Chemistry*, 59(1):72–118, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01174-7`.

Bayon:2021:UBT

[3193] L. Bayón, P. Fortuny Ayuso, and P. M. Suarez. Using the blow-up technique for a modified Lindemann mechanism. *Journal of Mathematical Chemistry*, 59(1):119–130, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01183-6`.

Ruiz:2021:IPC

[3194] Irene Luque Ruiz and Miguel Ángel Gómez-Nieto. Improvement the performance of the classification models of Cyclooxygenase-2 inhibitors using undersampling methods based on the rivality and reliability indexes. *Journal of Mathematical Chemistry*, 59(1):131–160, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01184-5`.

Amore:2021:ELC

[3195] Paolo Amore and Francisco M. Fernández. Energy levels of a coupled-rotors model. *Journal of Mathematical Chemistry*, 59(1):161–167, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01186-3`.

Baronas:2021:MCO

[3196] Romas Baronas, Juozas Kulys, and Linas Petkevicius. Modeling carbohydrates oxidation by oxygen catalyzed by bienzyme glucose dehydrogenase/laccase system immobilized into microreactor with carbon nanotubes. *Journal of Mathematical Chemistry*, 59(1):168–185, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL https://link.springer.com/article/10.1007/s10910-020-01187-2.

Shivhare:2021:UCQ

[3197] Meenakshi Shivhare, Pramod Chakravarthy Podila, and Devendra Kumar. A uniformly convergent quadratic B-spline collocation method for singularly perturbed parabolic partial differential equations with two small parameters. *Journal of Mathematical Chemistry*, 59(1):186–215, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01190-7.

Mungkasi:2021:NVO

[3198] Sudi Mungkasi. Numerical verification of the orders of accuracy of truncated asymptotic expansion solutions to the van der Pol equation. *Journal of Mathematical Chemistry*, 59(1):216–223, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01191-6.

Shokri:2021:NIH

[3199] Ali Shokri and Mohammad Mehdizadeh Khalsaraei. A new implicit high-order six-step singularly p-stable method for the numerical solution of Schrödinger equation. *Journal of Mathematical Chemistry*, 59(1):224–249, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01189-0.

Andova:2021:DBI

[3200] Vesna Andova, Martin Knor, and Riste Skrekovski. Distance based indices in nanotubical graphs: part 3. *Journal of Mathematical Chemistry*, 59(1):250–263, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01192-5.

Bille:2021:SCC

[3201] Artur Bille, Victor Buchstaber, and Evgeny Spodarev. Spectral clustering of combinatorial fullerene isomers based on their facet graph structure. *Journal of Mathematical Chemistry*, 59(1):264–288, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01193-4.

Fecteau:2021:RGG

[3202] Charles-Émile Fecteau, Frédéric Berthiaume, and Paul Andrew Johnson. Richardson–Gaudin geminal wavefunctions in a Slater determinant basis. *Journal of Mathematical Chemistry*, 59(1):289–301, January 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01197-0`.

Morales:2021:IQD

[3203] J. Morales, J. J. Peña, and J. García-Ravelo. On the improvement of q -deformed hyperbolic functions. *Journal of Mathematical Chemistry*, 59 (2):303–314, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01200-8`.

Balasubramanian:2021:CER

[3204] Krishnan Balasubramanian. Combinatorial enumeration of relativistic states of actinide dimers. *Journal of Mathematical Chemistry*, 59(2): 315–363, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01196-1`.

Belkic:2021:DNSa

[3205] Dzevad Belkić and Karen Belkić. Derivative NMR spectroscopy for J-coupled multiplet resonances using short time signals (0.5 KB) encoded at low magnetic field strengths (1.5T). Part I: water suppressed. *Journal of Mathematical Chemistry*, 59(2):364–404, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01198-z`.

Belkic:2021:DNSb

[3206] Dzevad Belkić and Karen Belkić. Derivative NMR spectroscopy for J-coupled multiplet resonances using short time signals (0.5KB) encoded at low magnetic field strengths (1.5T). Part II: Water unsuppressed. *Journal of Mathematical Chemistry*, 59(2):405–443, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01199-y`.

Buchowiecki:2021:ANB

[3207] Marcin Buchowiecki. Analytical non-Boltzmann vibrational distributions and their influence on vibrational partition function. *Journal of Mathematical Chemistry*, 59(2):444–458, February 2021. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01207-1.

Zhang:2021:MRL

[3208] Peng Zhang, Ping Li, and Alirio E. Rodrigues. Modeling Riemann–Liouville fractional differential equations for diffusion and reaction in fractal porous media. *Journal of Mathematical Chemistry*, 59(2):459–475, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01209-z.

Redzepovic:2021:CSS

[3209] Izudin Redzepović and Boris Furtula. Comparative study on structural sensitivity of eigenvalue-based molecular descriptors. *Journal of Mathematical Chemistry*, 59(2):476–487, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01202-6.

Torres-Vega:2021:SAF

[3210] Juan J. Torres-Vega, Gustavo E. Massaccesi, and Diego R. Alcoba. Symmetry-adapted formulation of the hybrid treatment resulting from the G-particle-hole hypervirial equation and equations of motion methods: a procedure for modeling solids. *Journal of Mathematical Chemistry*, 59(2):488–504, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01208-0.

Wang:2021:ESS

[3211] Yiting Wang and Jing Kong. Efficient spherical surface integration of Gauss functions in three-dimensional spherical coordinates and the solution for the modified Bessel function of the first kind. *Journal of Mathematical Chemistry*, 59(2):505–515, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01204-4.

Zhou:2021:ABS

[3212] Huihui Zhou, Yun Han, and Rui Yuan. Anticipated backward stochastic differential equations with non-Lipschitz coefficients. *Journal of Mathematical Chemistry*, 59(2):516–528, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01211-5.

Ren:2021:TPC

[3213] Haizhen Ren, Deqing Xu, and Weiling Yang. The Tutte polynomials of catacondensed benzenoid systems. *Journal of Mathematical Chemistry*, 59(2):529–541, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01205-3`.

Tian:2021:CNG

[3214] Ye Tian and Biao Zhao. On the Clar number of graphene fragment. *Journal of Mathematical Chemistry*, 59(2):542–553, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01214-w`.

Hariharan:2021:EOM

[3215] G. Hariharan, G. Swaminathan, and B. Sripathy. An efficient operational matrix approach for the solutions of Burgers' and fractional Burgers' equations using wavelets. *Journal of Mathematical Chemistry*, 59(2):554–573, February 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01206-2`.

Fackeldey:2021:ARS

[3216] Konstantin Fackeldey, Jonas Röhm, and Marcus Weber. Analyzing Raman spectral data without separabiliy assumption. *Journal of Mathematical Chemistry*, 59(3):575–596, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01201-7`.

Medvedev:2021:EFA

[3217] Maxim A. Medvedev and T. E. Simos. Efficient FinDiff algorithm with optimal phase properties for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 59(3):597–640, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01188-1`.

Wang:2021:NFM

[3218] Zenggui Wang and T. E. Simos. New FD methods with phase-lag and its derivatives equal to zero for periodic initial value problems. *Journal of Mathematical Chemistry*, 59(3):641–675, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01203-5`.

Rajan:2021:BPNa

[3219] R. Sundara Rajan, K. Jagadeesh Kumar, and Krishnan Balasubramanian. Biochemical and phylogenetic networks — I: hypertrees and corona products. *Journal of Mathematical Chemistry*, 59(3):676–698, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01194-3`.

Rajan:2021:BPNb

[3220] R. Sundara Rajan, A. Arul Shantrinal, and Krishnan Balasubramanian. Biochemical and phylogenetic networks — II: X-trees and phylogenetic trees. *Journal of Mathematical Chemistry*, 59(3):699–718, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-020-01195-2`.

Li:2021:APS

[3221] Guanru Li, Lily Li Liu, and Yi Wang. Analytic properties of sextet polynomials of hexagonal systems. *Journal of Mathematical Chemistry*, 59(3):719–734, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01213-x`.

Zuo:2021:GLF

[3222] Yuting Zuo. A gecko-like fractal receptor of a three-dimensional printing technology: a fractal oscillator. *Journal of Mathematical Chemistry*, 59 (3):735–744, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01212-y`.

Jia:2021:BDB

[3223] Ji-Teng Jia, Yu-Cong Yan, and Qi He. A block diagonalization based algorithm for the determinants of block k-tridiagonal matrices. *Journal of Mathematical Chemistry*, 59(3):745–756, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01216-8`.

Belhaj:2021:FAS

[3224] Skander Belhaj, Fahd Hcini, and Yulin Zhang. A fast algorithm for solving diagonally dominant symmetric quasi-pentadiagonal Toeplitz linear systems. *Journal of Mathematical Chemistry*, 59(3):757–774, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL https://link.springer.com/article/10.1007/s10910-021-01217-7.

Abreu-Blaya:2021:IGA

[3225] Ricardo Abreu-Blaya, Rosalio Reyes, and José M. Sigarreta. Inequalities on the generalized atom bond connectivity index. *Journal of Mathematical Chemistry*, 59(3):775–791, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01219-5.

Cassani:2021:BZT

[3226] Andrea Cassani, Alessandro Monteverde, and Marco Piumetti. Belousov–Zhabotinsky type reactions: the non-linear behavior of chemical systems. *Journal of Mathematical Chemistry*, 59(3):792–826, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01223-9.

Macias-Diaz:2021:ESN

[3227] Jorge E. Macías-Díaz, María G. Medina-Guevara, and Héctor Vargas-Rodríguez. Exact solutions of non-linear Klein–Gordon equation with non-constant coefficients through the trial equation method. *Journal of Mathematical Chemistry*, 59(3):827–839, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01220-y.

Hernandez:2021:PEH

[3228] Bryan S. Hernandez and Eduardo R. Mendoza. Positive equilibria of Hill-type kinetic systems. *Journal of Mathematical Chemistry*, 59(3):840–870, March 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01230-w.

Hayat:2021:AKN

[3229] Sakander Hayat. The anti-Kekulé number of graphs. *Journal of Mathematical Chemistry*, 59(4):871–941, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01221-x.

Kramer:2021:MDUa

[3230] Marie Kramer and Dieter Rautenbach. Minimum distance-unbalancedness of trees. *Journal of Mathematical Chemistry*, 59(4):942–950, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL

https://link.springer.com/article/10.1007/s10910-021-01228-4.

Lin:2021:NFD

[3231] Chia-Liang Lin and T. E. Simos. A new finite difference method with optimal phase and stability properties for problems in chemistry. *Journal of Mathematical Chemistry*, 59(4):951–984, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01215-9.

Cassam-Chenai:2021:SCP

[3232] Patrick Cassam-Chenaï and Gilles Lebeau. Smeared Coulomb potential orbitals: I — asymptotic expansion. *Journal of Mathematical Chemistry*, 59(4):985–1013, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01218-6.

Chaudhary:2021:TCN

[3233] Shalini Chaudhary, Abhay Chaudhary, and Tanmoy Chakraborty. Theoretical computation of normalised radii, density and global hardness as a function of orbital exponent. *Journal of Mathematical Chemistry*, 59 (4):1014–1028, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01224-8.

Carbo-Dorca:2021:GSP

[3234] Ramon Carbó-Dorca. Generalized scalar products in Minkowski metric spaces. *Journal of Mathematical Chemistry*, 59(4):1029–1045, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01229-3.

Qin:2021:DTM

[3235] Yupeng Qin and Qingjun Lou. Differential transform method for the solutions to some initial value problems in chemistry. *Journal of Mathematical Chemistry*, 59(4):1046–1053, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01225-7. See comment [3299].

Tikhonov:2021:MPC

[3236] N. A. Tikhonov, M. G. Tokmachev, and R. Kh. Khamizov. Modeling the process of capacitive deionization of solutions at supposing complex

structure of the pores of the electrodes. *Journal of Mathematical Chemistry*, 59(4):1054–1067, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01226-6`.

Shi:2021:SSS

[3237] Yao Shi, Qian Cao, and Yunfeng Jia. Steady-state solutions of the templator model in chemical self-replication. *Journal of Mathematical Chemistry*, 59(4):1068–1097, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01233-7`.

Cruz:2021:EVS

[3238] Roberto Cruz and Juan Rada. Extremal values of the Sombor index in unicyclic and bicyclic graphs. *Journal of Mathematical Chemistry*, 59 (4):1098–1116, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01232-8`.

Shahni:2021:NSS

[3239] Julee Shahni and Randhir Singh. Numerical solution of system of Emden–Fowler type equations by Bernstein collocation method. *Journal of Mathematical Chemistry*, 59(4):1117–1138, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01235-5`.

He:2021:HPM

[3240] Ji-Huan He and Yusry O. El-Dib. Homotopy perturbation method with three expansions. *Journal of Mathematical Chemistry*, 59(4): 1139–1150, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01237-3`.

Carbo-Dorca:2021:ACP

[3241] Ramon Carbó-Dorca. About the construction of probability hypercubes. *Journal of Mathematical Chemistry*, 59(4):1151–1154, April 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01227-5`.

Lin:2021:NMV

[3242] Chia-Liang Lin and T. E. Simos. A new method with vanished phase-lag and its derivatives of the highest order for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 59(5):1155–1200,

May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01222-w.

Medvedev:2021:NFN

[3243] Maxim A. Medvedev and T. E. Simos. A new FinDiff numerical scheme with phase-lag and its derivatives equal to zero for periodic initial value problems. *Journal of Mathematical Chemistry*, 59(5): 1201–1233, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-020-01210-6.

Nadeem:2021:LVI

[3244] Muhammad Nadeem and Ji-Huan He. He-Laplace variational iteration method for solving the nonlinear equations arising in chemical kinetics and population dynamics. *Journal of Mathematical Chemistry*, 59(5): 1234–1245, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01236-4. See comment [3312].

Aguilar-Sanchez:2021:ASS

[3245] R. Aguilar-Sánchez, J. A. Méndez-Bermúdez, and José M. Sigarreta. Analytical and statistical studies of Rodriguez–Velazquez indices. *Journal of Mathematical Chemistry*, 59(5):1246–1259, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01239-1.

Neumann:2021:SCT

[3246] Gunter Neumann. Some consequences of thermodynamic feasibility for chemical reaction networks. *Journal of Mathematical Chemistry*, 59(5): 1260–1282, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01231-9.

Borisov:2021:TSE

[3247] Milen Borisov and Svetoslav Markov. The two-step exponential decay reaction network: analysis of the solutions and relation to epidemiological SIR models with logistic and Gompertz type infection contact patterns. *Journal of Mathematical Chemistry*, 59(5):1283–1315, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01240-8.

Zhang:2021:NPD

[3248] Yaxian Zhang and Heping Zhang. Nice pairs of disjoint pentagons in fullerene graphs. *Journal of Mathematical Chemistry*, 59(5):1316–1331, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01242-6`.

Sylvia:2021:SNR

[3249] S. Vinolyn Sylvia, R. Joy Salomi, and Marwan Abukhaled. Solving nonlinear reaction-diffusion problem in electrostatic interaction with reaction-generated pH change on the kinetics of immobilized enzyme systems using Taylor series method. *Journal of Mathematical Chemistry*, 59 (5):1332–1347, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01241-7`.

Bermudo:2021:DNC

[3250] Sergio Bermudo, Robinson A. Higuita, and Juan Rada. Domination number of catacondensed hexagonal systems. *Journal of Mathematical Chemistry*, 59(5):1348–1367, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01243-5`.

Pasca:2021:ATB

[3251] Daniel Pasca, Cristina Stoica, and Cláudia Valls. Anisotropic two-body problem under the Buckingham potential. *Journal of Mathematical Chemistry*, 59(5):1368–1377, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01244-4`.

Cai:2021:HIE

[3252] Junqing Cai, Panpan Wang, and Linlin Zhang. Harary index of Eulerian graphs. *Journal of Mathematical Chemistry*, 59(5):1378–1394, May 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01246-2`.

Ma:2021:NEM

[3253] Yu-Yu Ma, Chia-Liang Lin, and T. E. Simos. A new economical method with eliminated phase-lag and its derivative for problems in chemistry. *Journal of Mathematical Chemistry*, 59(6):1395–1428, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL https://link.springer.com/article/10.1007/s10910-021-01238-2.

Theresal:2021:IEH

[3254] Santiagu Theresal, Antony Xavier, and S. Maria Jesu Raja. Induced H-packing k-partition problem in certain carbon based nanostructures. *Journal of Mathematical Chemistry*, 59(6):1429–1449, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01234-6.

Carbo-Dorca:2021:EED

[3255] Ramon Carbó-Dorca. Enfolding N-dimensional Euclidean spaces with N-dimensional spheres as a framework to define the structure of time foam. *Journal of Mathematical Chemistry*, 59(6):1450–1455, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01251-5.

Skakauskas:2021:MRN

[3256] V. Skakauskas and P. Katauskis. Modelling reduction of nitric oxide by hydrogen over supported catalysts. *Journal of Mathematical Chemistry*, 59(6):1456–1473, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01248-0.

Holba:2021:NLC

[3257] Pavel Holba. Nonexistence of local conservation laws for generalized Swift–Hohenberg equation. *Journal of Mathematical Chemistry*, 59(6):1474–1478, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01249-z.

Cortes:2021:FPA

[3258] J.-C. Cortés, A. Navarro-Quiles, and M.-D. Roselló. A full probabilistic analysis of a randomized kinetic model for reaction–deactivation of hydrogen peroxide decomposition with applications to real data. *Journal of Mathematical Chemistry*, 59(6):1479–1497, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01247-1.

Cebic:2021:MBI

[3259] Dejan Ćebić and Nebojsa M. Ralević. Mean-based iterative methods for finding multiple roots in nonlinear chemistry problems. *Journal of Math-*

ematical Chemistry, 59(6):1498–1519, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01253-3`.

Gutman:2021:RBG

[3260] Ivan Gutman. Relation between geometric-arithmetic and arithmetic-geometric indices. *Journal of Mathematical Chemistry*, 59(6):1520–1525, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01256-0`.

Rosenfeld:2021:CZE

[3261] Vladimir R. Rosenfeld and Yujun Yang. Close-to-zero eigenvalues of the rooted product of graphs. *Journal of Mathematical Chemistry*, 59 (6):1526–1535, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01250-6`.

Lal:2021:AFL

[3262] Shyam Lal and Priya Kumari. Approximation of functions of Lipschitz class and solution of Fokker–Planck equation by two-dimensional Legendre wavelet operational matrix. *Journal of Mathematical Chemistry*, 59 (6):1536–1550, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01257-z`.

Rosenfeld:2021:SVQ

[3263] Vladimir R. Rosenfeld. The spectrum of the vertex quadrangulation of a 4-regular toroidal graph and beyond. *Journal of Mathematical Chemistry*, 59(6):1551–1569, June 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01254-2`.

Li:2021:NMI

[3264] Xingyuan Li, Chia-Liang Lin, and T. E. Simos. A new method with improved phase-lag and stability properties for problems in quantum chemistry — an economical case. *Journal of Mathematical Chemistry*, 59(7): 1571–1602, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01245-3`.

Indulal:2021:GPP

[3265] Gopalapillai Indulal, Liju Alex, and Ivan Gutman. On graphs preserving PI index upon edge removal. *Journal of Mathematical Chemistry*, 59(7):

1603–1609, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01255-1`.

Swati:2021:UHW

[3266] Swati, Mandeep Singh, and Karanjeet Singh. Uniform Haar wavelet technique with Newton's method for a kind of derivative dependent SBVPs. *Journal of Mathematical Chemistry*, 59(7):1610–1637, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01259-x`.

Parmar:2021:EKG

[3267] Rajendrasinh H. Parmar and P. C. Vinodkumar. Eigensolution of the Klein–Gordon equation for modified Yukawa–Kratzer potential and its applications using parametric Nikiforov–Uvarov and SUSYQM method. *Journal of Mathematical Chemistry*, 59(7):1638–1703, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01258-y`.

Medvedeva:2021:ETSa

[3268] Marina A. Medvedeva and T. E. Simos. An economical two-step method with improved phase and stability properties for problems in chemistry. *Journal of Mathematical Chemistry*, 59(7):1704–1737, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01260-4`.

Mingliang:2021:NIE

[3269] Zheng Mingliang and T. E. Simos. A new improved economical finite difference method for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 59(7):1738–1766, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01252-4`.

He:2021:CFN

[3270] Xin He and Heping Zhang. Complete forcing numbers of hexagonal systems. *Journal of Mathematical Chemistry*, 59(7):1767–1784, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01261-3`.

Zhuk:2021:EPI

[3271] P. F. Zhuk and S. O. Karakhim. Extreme properties of the initial rate of the four-stage reaction of enzyme catalyzed ATP hydrolysis. *Journal of Mathematical Chemistry*, 59(7):1785–1807, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01262-2`.

Szabo:2021:GNG

[3272] Rebeka Szabó and Gábor Lente. General nucleation-growth type kinetic models of nanoparticle formation: possibilities of finding analytical solutions. *Journal of Mathematical Chemistry*, 59(7):1808–1821, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01265-z`.

Flores-Gallegos:2021:EQR

[3273] N. Flores-Gallegos. q-Rényi's entropy as a possible measure of electron correlation. *Journal of Mathematical Chemistry*, 59(7):1822–1835, August 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01268-w`.

Swaminathan:2021:NSC

[3274] G. Swaminathan, G. Hariharan, and S. Bharatwaja. A new spectral collocation method for solving Bratu-type equations using Genocchi polynomials. *Journal of Mathematical Chemistry*, 59(8):1837–1850, September 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01264-0`.

Carbo-Dorca:2021:EFL

[3275] Ramon Carbó-Dorca, Sebastián Reyes, and Alfonso Niño. Extension of Fermat's last theorem in Minkowski natural spaces. *Journal of Mathematical Chemistry*, 59(8):1851–1863, September 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01267-x`.

Nanni:2021:SSE

[3276] Luca Nanni. Solving the Schrödinger equation of an electron in a periodic crystal potential through elliptic functions. *Journal of Mathematical Chemistry*, 59(8):1864–1874, September 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01269-9`.

Carbo-Dorca:2021:EMS

[3277] Ramon Carbó-Dorca and Tanmoy Chakraborty. Extended Minkowski spaces, zero norms, and Minkowski hypersurfaces. *Journal of Mathematical Chemistry*, 59(8):1875–1879, September 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01266-y`.

Medvedev:2021:TSM

[3278] Maxim A. Medvedev and T. E. Simos. Two-step method with vanished phase-lag and its derivatives for problems in quantum chemistry: an economical case. *Journal of Mathematical Chemistry*, 59(8):1880–1916, September 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01263-1`.

Tunc:2021:SPT

[3279] Huseyin Tunc and Murat Sari. A stability preserved time-integration method for nonlinear advection–diffusion–reaction processes. *Journal of Mathematical Chemistry*, 59(8):1917–1937, September 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01271-1`.

Medvedeva:2021:ETSb

[3280] Marina A. Medvedeva and T. E. Simos. An economical two-step method with optimal phase and stability properties for problems in chemistry. *Journal of Mathematical Chemistry*, 59(8):1938–1975, September 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01270-2`.

Roul:2021:ENA

[3281] Pradip Roul, Trishna Kumari, and V. M. K. Prasad Goura. An efficient numerical approach for solving a general class of nonlinear singular boundary value problems. *Journal of Mathematical Chemistry*, 59(9):1977–1993, October 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01279-7`.

Hariharan:2021:WMS

[3282] G. Hariharan and S. Padma. Wavelet method for steady state immobilized enzyme kinetic model: an operational matrix approach. *Journal of Mathematical Chemistry*, 59(9):1994–2008, October 2021. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01272-0`.

Tiebekabe:2021:LFL

[3283] Pagdame Tiebekabe and Ismaïla Diouf. Linear forms in logarithms and the mathematical method of diophantine equations: applications in chemistry and physics. *Journal of Mathematical Chemistry*, 59(9): 2009–2020, October 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01274-y`. See correction [3716].

Alonso:2021:AMH

[3284] M. M. Canedo Alonso, Jaime González Cuadra, and J. L. González-Hernández. ANN-MATOPT hybrid algorithm: determination of kinetic and non-kinetic parameters in different reaction mechanisms. *Journal of Mathematical Chemistry*, 59(9):2021–2048, October 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01275-x`.

Aghili:2021:BRA

[3285] Alireza Aghili, Nadezda Sukhorukova, and Julien Ugon. Bivariate rational approximations of the general temperature integral. *Journal of Mathematical Chemistry*, 59(9):2049–2062, October 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01273-z`.

Anderson:2021:DZR

[3286] David F. Anderson and Tung D. Nguyen. Deficiency zero for random reaction networks under a stochastic block model framework. *Journal of Mathematical Chemistry*, 59(9):2063–2097, October 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01278-8`.

Brizard:2021:ALC

[3287] Alain J. Brizard and Samuel M. Berry. Asymptotic limit-cycle analysis of oscillating chemical reactions. *Journal of Mathematical Chemistry*, 59(9): 2098–2132, October 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01276-w`.

Belkic:2021:EVD

[3288] Dzevad Belkić and Karen Belkić. *In vivo* derivative NMR spectroscopy for simultaneous improvements of resolution and signal-to-noise-ratio:

Case study, Glioma. *Journal of Mathematical Chemistry*, 59(9):2133–2178, October 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01280-0`.

Molski:2021:MUC

[3289] Marcin Molski. Minimum-uncertainty coherent states of the hyperbolic and trigonometric Rosen–Morse oscillators. *Journal of Mathematical Chemistry*, 59(9):2179–2191, October 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01281-z`.

Pawlak:2021:AAS

[3290] Mariusz Pawlak and Marcin Stachowiak. Analytical angular solutions for the atom-diatom interaction potential in a basis set of products of two spherical harmonics: two approaches. *Journal of Mathematical Chemistry*, 59(10):2193–2205, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01282-y`.

Al:2021:SRA

[3291] Pembe Ipek Al and Zameddin I. Ismailov. On the spectral radius of antidiagonal block operator matrices. *Journal of Mathematical Chemistry*, 59(10):2206–2217, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01286-8`.

Belkic:2021:HRV

[3292] Dzevad Belkić and Karen Belkić. High-resolution at 3T for in vivo derivative NMR spectroscopy in medical diagnostics of ovarian tumor: exact quantification by shape estimations. *Journal of Mathematical Chemistry*, 59(10):2218–2260, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01283-x`.

Kramer:2021:MDUb

[3293] Marie Kramer and Dieter Rautenbach. Maximally distance-unbalanced trees. *Journal of Mathematical Chemistry*, 59(10):2261–2269, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01287-7`.

Egawa:2021:NMF

[3294] Tsuyoshi Egawa. A new mathematical formula to link near equilibrium relaxation kinetics and conformational selection steps in enzymatic reactions. *Journal of Mathematical Chemistry*, 59(10):2270–2283, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01288-6`.

Nanni:2021:NAS

[3295] Luca Nanni. A new approach to solve the Schrödinger equation with an anharmonic sextic potential. *Journal of Mathematical Chemistry*, 59(10):2284–2293, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01289-5`. See comment [3313].

Dhont:2021:MGF

[3296] Guillaume Dhont, Patrick Cassam-Chenaï, and Frédéric Patras. Molien generating functions and integrity bases for the action of the SO(3) and O(3) groups on a set of vectors. *Journal of Mathematical Chemistry*, 59(10):2294–2326, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01277-9`.

Shahni:2021:BGW

[3297] Julee Shahni and Randhir Singh. Bernstein and Gegenbauer-wavelet collocation methods for Bratu-like equations arising in electrospinning process. *Journal of Mathematical Chemistry*, 59(10):2327–2343, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01290-y`.

Fu:2021:SCD

[3298] Xiaoxue Fu, Ranchao Wu, and Hongxia Liu. Spatiotemporal complexity in a diffusive Brusselator model. *Journal of Mathematical Chemistry*, 59(10):2344–2367, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01291-x`.

Fernandez:2021:CDT

[3299] Francisco M. Fernández and Javier Garcia. Comment on "Differential transform method for the solutions to some initial value problems in chemistry". *Journal of Mathematical Chemistry*, 59(10):2368–2372, November 2021. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01285-9. See [3235].

Medvedev:2022:PFS

[3300] Maxim A. Medvedev and T. E. Simos. A phase-fitting singularly p-stable economical two-step method for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 60(1):1–48, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01284-w.

Faught:2022:SFG

[3301] Nolan Faught, Mark Kempton, and Adam Knudson. A 1-separation formula for the graph Kemeny constant and Braess edges. *Journal of Mathematical Chemistry*, 60(1):49–69, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01294-8.

Medvedeva:2022:SST

[3302] Marina A. Medvedeva and T. E. Simos. A singularly P-stable two-step method with improved characteristics for problems in chemistry. *Journal of Mathematical Chemistry*, 60(1):70–91, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01292-w.

Doktorov:2022:LTS

[3303] Alexander B. Doktorov. Long-term and short-term asymptotes of reaction rate constants in the presence of reactivity anisotropy. *Journal of Mathematical Chemistry*, 60(1):92–127, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01295-7.

Roul:2022:QTB

[3304] Pradip Roul and Trishna Kumari. A quartic trigonometric B-spline collocation method for a general class of nonlinear singular boundary value problems. *Journal of Mathematical Chemistry*, 60(1):128–144, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01293-9.

Perelman:2022:CCQ

[3305] Carlos Castro Perelman and Ramon Carbó-Dorca. The Collatz conjecture and the quantum mechanical harmonic oscillator. *Journal of Mathematical Chemistry*, 60(1):145–160, January 2022. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01296-6.

Knowles:2022:DPG

[3306] Peter J. Knowles. The determination of point groups from imprecise molecular geometries. *Journal of Mathematical Chemistry*, 60(1): 161–171, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01302-x.

Dabulyte-Bagdonaviciene:2022:IDD

[3307] Jurgita Dabulyte-Bagdonaviciene, Anatolij Neciporenko, and Aivaras Kareiva. Influence of different diffusion rates of reaction reagents on the synthesis of yttrium aluminium garnet (YAG). *Journal of Mathematical Chemistry*, 60(1):172–183, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01303-w.

Li:2022:EAG

[3308] Chen Li. Exact analytical ground state solution of 1D H_2^+ with soft Coulomb potential. *Journal of Mathematical Chemistry*, 60(1):184–194, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01304-9.

Johnston:2022:AMA

[3309] Matthew D. Johnston. Analysis of mass-action systems by split network translation. *Journal of Mathematical Chemistry*, 60(1):195–218, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01299-3.

Zlatev:2022:EIA

[3310] Zahari Zlatev, Ivan Dimov, and Ágnes Havasi. Efficient implementation of advanced Richardson Extrapolation in an atmospheric chemical scheme. *Journal of Mathematical Chemistry*, 60(1):219–238, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01300-z.

Flores-Gallegos:2022:RDC

[3311] N. Flores-Gallegos. Rényi's divergence as a chemical similarity criterion. *Journal of Mathematical Chemistry*, 60(1):239–254, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL https://link.springer.com/article/10.1007/s10910-021-01307-6.

Fernandez:2022:CLV

[3312] Francisco M. Fernández. Comment on "He-Laplace variational iteration method for solving the nonlinear equations arising in chemical kinetics and population dynamics". *Journal of Mathematical Chemistry*, 60(1): 255–259, January 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01297-5. See [3244].

Fernandez:2022:CNA

[3313] Francisco M. Fernández. Comment on "A new approach to solve the Schrödinger equation with an anharmonic sextic potential". *Journal of Mathematical Chemistry*, 60(2):261–266, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01308-5. See [3295].

Mihalka:2022:GFQ

[3314] Zs. É. Mihálka, M. Nooijen, and P. R. Surján. The γ function in quantum theory II. Mathematical challenges and paradoxa. *Journal of Mathematical Chemistry*, 60(2):267–282, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01311-w.

Carbo-Dorca:2022:SHV

[3315] Ramon Carbó-Dorca. Shadows' hypercube, vector spaces, and non-linear optimization of QSPR procedures. *Journal of Mathematical Chemistry*, 60(2):283–310, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01301-y.

Medvedeva:2022:TSM

[3316] Marina A. Medvedeva and T. E. Simos. A two-step method singularly p-stable with improved properties for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 60(2):311–336, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01298-4.

Zhao:2022:TDA

[3317] Yan Zhao, Yanying Wang, and Huiyun Han. Topological data analysis for the energy and stability of endohedral metallofullerenes. *Journal of*

Mathematical Chemistry, 60(2):337–352, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01309-4.

Carbo-Dorca:2022:DUM

[3318] Ramon Carbó-Dorca. Determination of unknown molecular properties in molecular spaces. *Journal of Mathematical Chemistry*, 60(2):353–359, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01305-8.

Kumari:2022:AEB

[3319] Varsha Kumari, Tanupriya Singh, and Tanmoy Chakraborty. Atomic electronegativity based on hardness and floating spherical Gaussian orbital approach. *Journal of Mathematical Chemistry*, 60(2):360–372, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01306-7.

Belkic:2022:VPMa

[3320] Dzevad Belkić and Karen Belkić. In vitro proton magnetic resonance spectroscopy at 14T for benign and malignant ovary: Part I, signal processing by the nonparametric fast Padé transform. *Journal of Mathematical Chemistry*, 60(2):373–416, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01314-7.

Vasicek:2022:SNE

[3321] Jakub Vasícek. Symmetry nonintegrability for extended $K(m, n, p)$ equation. *Journal of Mathematical Chemistry*, 60(2):417–422, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01312-9.

Kouibia:2022:RAM

[3322] Abdelouahed Kouibia and Miguel Pasadas. Reconstruction approximating method by biquadratic splines of offset surfaces holes. *Journal of Mathematical Chemistry*, 60(2):423–439, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-021-01322-7.

Carbo-Dorca:2022:AEQ

[3323] Ramon Carbó-Dorca and Debraj Nath. Average energy and quantum similarity of a time dependent quantum system subject to Pöschl–

Teller potential. *Journal of Mathematical Chemistry*, 60(2):1–21, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01318-3`.

Elias-Zuniga:2022:FEM

[3324] Alex Elías-Zúñiga, Oscar Martínez-Romero, and Luis Manuel Palacios-Pineda. Fractal equation of motion of a non-Gaussian polymer chain: investigating its dynamic fractal response using an ancient Chinese algorithm. *Journal of Mathematical Chemistry*, 60(2):461–473, February 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01310-x`.

Generalov:2022:TSS

[3325] Dmitry Generalov, Ekaterina Tsvetova, and T. E. Simos. A two-step singularly p-stable method with high phase and large stability properties for problems in chemistry. *Journal of Mathematical Chemistry*, 60 (3):475–501, March 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01313-8`.

Rosenfeld:2022:IEG

[3326] Vladimir R. Rosenfeld. The inertia and energy gap of a vertex-decorated graph with identically weighted 'internal' edges and beyond. *Journal of Mathematical Chemistry*, 60(3):502–513, March 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01317-4`.

Roul:2022:FNS

[3327] Pradip Roul and V. M. K. Prasad Goura. A fast numerical scheme for solving singular boundary value problems arising in various physical models. *Journal of Mathematical Chemistry*, 60(3):514–541, March 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01316-5`.

Lin:2022:HPE

[3328] Haoyu Lin, Heng Zhang, and Shuya Liu. On the HOMFLY polynomials of even trigonal bipyramid links. *Journal of Mathematical Chemistry*, 60 (3):542–554, March 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01315-6`.

Fernandez:2022:RHO

[3329] Francisco M. Fernández. The rotating harmonic oscillator revisited. *Journal of Mathematical Chemistry*, 60(3):555–561, March 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01320-9`.

Conza:2022:MSD

[3330] Adelaida O. Conza and Álvaro L. de Bortoli. Modeling and simulation of diffusion flames of H_2 and methyl formate using the REDIM method. *Journal of Mathematical Chemistry*, 60(3):562–580, March 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01319-2`.

Carbo-Dorca:2022:NHS

[3331] Ramon Carbó-Dorca. A naïve HMO study of the Casimir effect. *Journal of Mathematical Chemistry*, 60(3):581–585, March 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01323-6`.

Murugan:2022:ASR

[3332] R. Murugan. Approximate solutions to the response time problems of transcription autoregulatory gene networks. *Journal of Mathematical Chemistry*, 60(3):586–604, March 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01324-5`.

Sun:2022:ESA

[3333] Guo-Hua Sun, Qian Dong, and Shi-Hai Dong. Exact solutions of an asymmetric double well potential. *Journal of Mathematical Chemistry*, 60(4):605–612, April 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01328-9`.

Houjou:2022:FPB

[3334] Hirohiko Houjou and Masataka Seshimo. Formulation of a phonon band calculation for molecular crystals using a coarse-grained coordinate approach under periodic boundary conditions. *Journal of Mathematical Chemistry*, 60(4):613–636, April 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01327-w`.

Lin:2022:MCP

[3335] Chia-Liang Lin and T. E. Simos. A multistep conditionally p-stable method with phase properties of high order for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 60(4):637–665, April 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01326-x`.

He:2022:CFN

[3336] Xin He and Heping Zhang. Complete forcing numbers of hexagonal systems II. *Journal of Mathematical Chemistry*, 60(4):666–680, April 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01330-1`.

Celebre:2022:CSB

[3337] Giorgio Celebre. Chiral symmetry breaking: Frank model for the evolution of homochirality described by population dynamics. *Journal of Mathematical Chemistry*, 60(4):681–694, April 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01329-8`.

Abraham:2022:GEE

[3338] Jessie Abraham, Micheal Arockiaraj, and Krishnan Balasubramanian. Graph entropies, enumeration of circuits, walks and topological properties of three classes of isoreticular metal organic frameworks. *Journal of Mathematical Chemistry*, 60(4):695–732, April 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-021-01321-8`.

Amrutha:2022:IRD

[3339] P. Amrutha, T. Bakkyaraj, and T. Geetha. Induced representations of dihedral groups (D_n) from its subgroups and to the symmetric groups (S_n): Applications to nanotubes, Gel'fand states tableaus and spectroscopy. *Journal of Mathematical Chemistry*, 60(4):733–751, April 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01325-y`.

Mei:2022:MLF

[3340] Suyu Mei. A machine learning framework for predicting synergistic and antagonistic drug combinatorial efficacy. *Journal of Mathematical*

Chemistry, 60(4):752–769, April 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01331-0`.

Liu:2022:SIR

[3341] Hechao Liu, Ivan Gutman, and Yufei Huang. Sombor index: review of extremal results and bounds. *Journal of Mathematical Chemistry*, 60 (5):771–798, May 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01333-y`.

Hernandez:2022:WRC

[3342] Bryan S. Hernandez and Eduardo R. Mendoza. Weakly reversible CF-decompositions of chemical kinetic systems. *Journal of Mathematical Chemistry*, 60(5):799–829, May 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01332-z`.

Chatterjee:2022:ERM

[3343] Supriya Chatterjee. On the exact revival of Morse oscillator wave packets. *Journal of Mathematical Chemistry*, 60(5):830–840, May 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01336-9`.

Besya:2022:TQS

[3344] Azimberdy Besya and Shodhan Rao. The total quasi-steady-state for multiple alternative substrate reactions. *Journal of Mathematical Chemistry*, 60(5):841–861, May 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01339-6`.

Archibald:2022:LDV

[3345] M. Archibald, S. Currie, and M. Nowaczyk. Locating a double vacancy or Stone–Wales point defect on a hexagonal quantum grid. *Journal of Mathematical Chemistry*, 60(5):862–873, May 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01337-8`.

Rosenfeld:2022:UBG

[3346] Vladimir R. Rosenfeld. On using Brandt groupoids in physicochemical research. *Journal of Mathematical Chemistry*, 60(5):874–890, May 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL https://link.springer.com/article/10.1007/s10910-022-01335-w.

Kothiyal:2022:ICS

[3347] Manuja Kothiyal, Santosh Kumar, and N. Sukumar. Investigation of chemical space networks using graph measures and random matrix theory. *Journal of Mathematical Chemistry*, 60(5):891–914, May 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01341-y.

Yuan:2022:MDD

[3348] Youyang Yuan, Hui Lv, and Qiang Zhang. Molecular device design based on chemical reaction networks: state feedback controller, static pre-filter, addition gate control system and full-dimensional state observer. *Journal of Mathematical Chemistry*, 60(5):915–935, May 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01340-z.

Medvedeva:2022:MMO

[3349] Marina A. Medvedeva and T. E. Simos. A multistep method with optimal phase and stability properties for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 60(6):937–968, June 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01342-x.

Huang:2022:MGA

[3350] Daniel Huang, Chong Teng, and Jean-Baptiste Tristan. mad-GP: automatic differentiation of Gaussian processes for molecules and materials. *Journal of Mathematical Chemistry*, 60(6):969–1000, June 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01334-x.

Szederkenyi:2022:PSC

[3351] Gábor Szederkényi, Bernadett Ács, and Mihály A. Vághy. Persistence and stability of a class of kinetic compartmental models. *Journal of Mathematical Chemistry*, 60(6):1001–1020, June 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01338-7.

Geneson:2022:PNT

[3352] Jesse Geneson and Shen-Fu Tsai. Peripherality in networks: theory and applications. *Journal of Mathematical Chemistry*, 60(6):1021–1079,

June 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01345-8.

Chung:2022:LTM

[3353] Wonsang Chung, Yeounju Kim, and Jeongmin Kwon. Laplace transform method in one dimensional quantum mechanics on the semi infinite axis. *Journal of Mathematical Chemistry*, 60(6):1080–1088, June 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01348-5.

Nath:2022:AST

[3354] Debraj Nath and Ramon Carbó-Dorca. Analysis of solutions of time-dependent Schrödinger equation of a particle trapped in a spherical box. *Journal of Mathematical Chemistry*, 60(6):1089–1106, June 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01350-x.

Kaya:2022:RRM

[3355] Rusen Kaya and Hasan Taseli. A Rayleigh–Ritz method for numerical solutions of linear Fredholm integral equations of the second kind. *Journal of Mathematical Chemistry*, 60(6):1107–1129, June 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01344-9.

Mandal:2022:DEC

[3356] Bholanath Mandal and Douglas J. Klein. Dendrimer eigen-characteristics. *Journal of Mathematical Chemistry*, 60(7):1131–1162, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01353-8.

Nishiyama:2022:RPA

[3357] Takahiro Nishiyama. Rod-packing arrangements of invariant tori in solenoidal vector fields with cubic symmetries. *Journal of Mathematical Chemistry*, 60(7):1163–1199, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01349-4.

Belkic:2022:VPMb

[3358] Dzevad Belkić and Karen Belkić. In vitro proton magnetic resonance spectroscopy at 14T for benign and malignant ovary: Part II, signal

processing by the parametric fast Padé transform. *Journal of Mathematical Chemistry*, 60(7):1200–1271, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01357-4`.

Serna-Reyes:2022:CAC

[3359] Adán Serna-Reyes, Jorge E. Macías-Díaz, Armando Gallegos, and Nuria Reguera. CMMSE: analysis and comparison of some numerical methods to solve a nonlinear fractional Gross–Pitaevskii system. *Journal of Mathematical Chemistry*, 60(7):1272–1286, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01360-9`.

Levay:2022:SEF

[3360] Péter Lévay. Special entangled fermionic systems and exceptional symmetries. *Journal of Mathematical Chemistry*, 60(7):1287–1313, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01358-3`.

Deswal:2022:TDH

[3361] Komal Deswal, Devendra Kumar, and J. Vigo-Aguiar. Three-dimensional Haar wavelet method for singularly perturbed elliptic boundary value problems on non-uniform meshes. *Journal of Mathematical Chemistry*, 60(7):1314–1336, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01359-2`.

Slevinsky:2022:CFT

[3362] Richard M. Slevinsky and Hassan Safouhi. Compact formulae for three-center nuclear attraction integrals over exponential type functions. *Journal of Mathematical Chemistry*, 60(7):1337–1355, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01362-7`.

Khari:2022:ENT

[3363] Kartikay Khari and Vivek Kumar. An efficient numerical technique for solving nonlinear singularly perturbed reaction diffusion problem. *Journal of Mathematical Chemistry*, 60(7):1356–1382, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01365-4`.

Medvedev:2022:PFF

[3364] Maxim A. Medvedev and T. E. Simos. A phase-fitting and first derivative phase-fitting singularly P-stable economical two-step method for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 60(7): 1383–1404, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01352-9`.

Flores-Gallegos:2022:IBS

[3365] N. Flores-Gallegos. On the information balance in a simple chemical process. *Journal of Mathematical Chemistry*, 60(7):1405–1421, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01366-3`.

Laguna:2022:ITS

[3366] Humberto G. Laguna, Saúl J. C. Salazar, and Robin P. Sagar. Information theoretical statistical discrimination measures for electronic densities. *Journal of Mathematical Chemistry*, 60(7):1422–1444, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01363-6`.

Miroshnichenko:2022:TIT

[3367] Taisia Miroshnichenko, Vladimir Gubernov, Sergey Minaev, and Andrey Polezhaev. Thermal interaction in two-layered solid fuel system. *Journal of Mathematical Chemistry*, 60(7):1445–1460, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01346-7`. See correction [3368].

Miroshnichenko:2022:CTI

[3368] Taisia Miroshnichenko, Vladimir Gubernov, Sergey Minaev, and Andrey Polezhaev. Correction to: Thermal interaction in two-layered solid fuel system. *Journal of Mathematical Chemistry*, 60(7):1461, August 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01378-z`. See [3367].

Kumar:2022:EOM

[3369] Saurabh Kumar, Vikas Gupta, and J. F. Gómez-Aguilar. An efficient operational matrix technique to solve the fractional order non-local boundary value problems. *Journal of Mathematical Chemistry*, 60(8):1463–

1479, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01368-1`.

Sun:2022:PFF

[3370] Bin Sun, Chia-Liang Lin, and T. E. Simos. A phase-fitting, first and second derivatives phase-fitting singularly P-stable economical two-step method for problems in chemistry. *Journal of Mathematical Chemistry*, 60(8):1480–1504, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01361-8`.

Saloni:2022:CAE

[3371] Saloni, Dimple Kumari, Hiteshi Tandon, Martín Labarca, and Tanmoy Chakraborty. Computation of atomic electronegativity values using atomic and covalent potential: a FSGO based study. *Journal of Mathematical Chemistry*, 60(8):1505–1520, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01376-1`.

Cebic:2022:ECO

[3372] Dejan Ćebić and Nebojsa M. Ralević. An efficient class of optimal sixteenth-order root-finding methods and their basins of attraction. *Journal of Mathematical Chemistry*, 60(8):1521–1541, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01371-6`.

Poulsen:2022:PSR

[3373] Felipe Poulsen, Thorsten Hansen, and Matthew G. Reuter. Predicting slow relaxation timescales in open quantum systems. *Journal of Mathematical Chemistry*, 60(8):1542–1554, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01367-2`.

Garcia-Merino:2022:SME

[3374] José Carlos García-Merino, Carmen Calvo-Jurado, and Enrique García-Macías. Surrogate modeling of the effective elastic properties of spherical particle-reinforced composite materials. *Journal of Mathematical Chemistry*, 60(8):1555–1570, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01375-2`.

Balasubramanian:2022:TCE

[3375] Krishnan Balasubramanian and Ramon Carbó-Dorca. Three conjectures on extended twin primes and the existence of isoboolean and singular primes inspired by relativistic quantum computing. *Journal of Mathematical Chemistry*, 60(8):1571–1583, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01364-5`.

Roul:2022:NAS

[3376] Pradip Roul. A novel approach for solving nonlinear singular boundary value problems arising in various physical models. *Journal of Mathematical Chemistry*, 60(8):1584–1609, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01369-0`.

Li:2022:MIU

[3377] Genyuan Li. Moment independent uncertainty importance measure for stochastic systems based on Gaussian process. *Journal of Mathematical Chemistry*, 60(8):1610–1631, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01372-5`.

Lin:2022:PFF

[3378] Chia-Liang Lin and T. E. Simos. A phase-fitting, first, second and third derivatives phase-fitting singularly P-stable economical two-step method for problems in quantum chemistry. *Journal of Mathematical Chemistry*, 60(8):1632–1657, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01373-4`.

Jia:2022:IBD

[3379] Ji-Teng Jia, Jie Wang, Ting-Feng Yuan, Kai-Kai Zhang, and Bao-Ming Zhong. An incomplete block-diagonalization approach for evaluating the determinants of bordered k -tridiagonal matrices. *Journal of Mathematical Chemistry*, 60(8):1658–1673, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01377-0`.

Turulski:2022:SSC

[3380] Jan Turulski. On self-similar chemical structures, once again. *Journal of Mathematical Chemistry*, 60(8):1674–1694, September 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01370-7`.

Jia:2022:DFA

[3381] Ji-Teng Jia, Jie Wang, Qi He, and Yu-Cong Yan. A division-free algorithm for numerically evaluating the determinant of a specific quasi-tridiagonal matrix. *Journal of Mathematical Chemistry*, 60(9):1695–1706, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01386-z`.

Moisset:2022:PCH

[3382] Jean-David Moisset, Laurie Carrier, and Paul Andrew Johnson. Pertubative corrections for Hartree–Fock-like algebraic Bethe ansatz analogue. *Journal of Mathematical Chemistry*, 60(9):1707–1724, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01385-0`.

Chan:2022:TDL

[3383] Yue Chan, Ruidi Song, Rumiao Lin, Daoju Cai, and Shern-Long Lee. Time-dependent Langevin modeling and Monte–Carlo simulations of diffusion in one-dimensional ion channels. *Journal of Mathematical Chemistry*, 60(9):1725–1738, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01391-2`.

Apagyi:2022:DAA

[3384] B. Apagyi. Determination of α–α interaction from experiment. *Journal of Mathematical Chemistry*, 60(9):1739–1749, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01382-3`.

Andersons:2022:AES

[3385] Tomass Andersons, Mathias Sawall, and Klaus Neymeyr. Analytical enclosure of the set of solutions of the three-species multivariate curve resolution problem. *Journal of Mathematical Chemistry*, 60(9):1750–1780, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01380-5`.

Kazmierczak:2022:PSN

[3386] Anna Ka

zmierczak and Aleksandra Orpel. Positive solutions to the nonlinear reactor model by variational iteration method. *Journal of Mathematical Chemistry*, 60(9):1781–1799, October 2022. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01392-1.

FerreiraFlorindo:2022:DMW

[3387] Caio César Ferreira Florindo, Christina Papenfuss, and Adalberto Bono Maurizio Sacchi Bassi. On the description of the microdomains within carbon fiber precursory mesophase pitch: a mesoscopic continuum approach. *Journal of Mathematical Chemistry*, 60(9):1800–1818, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01389-w.

Nath:2022:SUA

[3388] Debraj Nath. Study of uncertainty, average energy, and thermodynamic quantities of the time dependent quantum system. *Journal of Mathematical Chemistry*, 60(9):1819–1839, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01388-x.

Flores-Gallegos:2022:PGS

[3389] N. Flores-Gallegos. A possible generalization Shannon's entropy using q-calculus. *Journal of Mathematical Chemistry*, 60(9):1840–1853, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01394-z.

Carballosa:2022:CPA

[3390] Walter Carballosa, Ana Granados, José Antonio Méndez Bermúdez, Domingo Pestana, and Ana Portilla. Computational properties of the arithmetic–geometric index. *Journal of Mathematical Chemistry*, 60(9):1854–1871, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01390-3.

Singh:2022:SBP

[3391] Satpal Singh and Devendra Kumar. Spline-based parameter-uniform scheme for fourth-order singularly perturbed differential equations. *Journal of Mathematical Chemistry*, 60(9):1872–1902, October 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01393-0.

Bradly:2022:CSL

[3392] C. J. Bradly and A. L. Owczarek. Critical scaling of lattice polymers confined to a box without endpoint restriction. *Journal of Mathemati-*

cal Chemistry, 60(10):1903–1920, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01387-y`.

Diaz-Marin:2022:GDS

[3393] Homero G. Díaz-Marín, Francisco J. López-Hernández, and Osvaldo Osuna. Global dynamics of solutions for enzyme catalysed models with almost periodic oscillatory input. *Journal of Mathematical Chemistry*, 60(10):1921–1929, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01396-x`.

Purohit:2022:SMY

[3394] Kaushal R. Purohit, Rajendrasinh H. Parmar, and Ajay Kumar Rai. Solution of the modified Yukawa–Kratzer potential under influence of the external fields and its thermodynamic properties. *Journal of Mathematical Chemistry*, 60(10):1930–1982, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01397-w`.

Song:2022:URM

[3395] Qingfei Song, Xingyu Zhang, Zekai Miao, Qiuyu Zhang, and Qingyong Meng. Unified regression model in fitting potential energy surfaces for quantum dynamics. *Journal of Mathematical Chemistry*, 60(10):1983–2012, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01400-4`.

Choi:2022:CSG

[3396] Howon Choi, Hyoungjun Kim, and Sungjong No. Chirality for simple graphs of size up to 12. *Journal of Mathematical Chemistry*, 60(10):2013–2028, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01398-9`.

Kumari:2022:SMB

[3397] Archna Kumari and V. K. Kukreja. Shishkin mesh based septic Hermite interpolation algorithm for time-dependent singularly perturbed convection–diffusion models. *Journal of Mathematical Chemistry*, 60(10):2029–2053, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01399-8`.

Tiwari:2022:WSS

[3398] Diksha Tiwari, Amit K. Verma, and Carlo Cattani. Wavelet solution of a strongly nonlinear Lane–Emden equation. *Journal of Mathematical Chemistry*, 60(10):2054–2080, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01401-3`.

Ali:2022:ABS

[3399] Akbar Ali, Boris Furtula, Izudin Redžepović, and Ivan Gutman. Atom-bond sum-connectivity index. *Journal of Mathematical Chemistry*, 60 (10):2081–2093, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01403-1`.

Lin:2022:PFS

[3400] Chia-Liang Lin and T. E. Simos. A phase-fitting singularly P-stable cost-effective two-step method for solving chemistry problems. *Journal of Mathematical Chemistry*, 60(10):2094–2124, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01395-y`.

Baldonedo:2022:CNA

[3401] Jacobo Baldonedo, José R. Fernández, Abraham Segade, and Sofía Suárez. CMMSE: numerical analysis of a chemical targeting model. *Journal of Mathematical Chemistry*, 60(10):2125–2138, November 2022. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01404-0`.

Fernandez:2023:TCP

[3402] Francisco M. Fernández. The truncated Coulomb potential revisited. *Journal of Mathematical Chemistry*, 61(1):1–6, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01405-z`.

Manzhos:2023:OHG

[3403] Sergei Manzhos and Manabu Ihara. Optimization of hyperparameters of Gaussian process regression with the help of a low-order high-dimensional model representation: application to a potential energy surface. *Journal of Mathematical Chemistry*, 61(1):7–20, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01407-x`.

Choudhary:2023:SOC

[3404] Renu Choudhary, Devendra Kumar, and Satpal Singh. Second-order convergent scheme for time-fractional partial differential equations with a delay in time. *Journal of Mathematical Chemistry*, 61(1):21–46, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01409-9`.

Singh:2023:DMS

[3405] Abhishek Kumar Singh and Mani Mehra. Difference methods for stochastic space fractional diffusion equation driven by additive space-time white noise via Wong–Zakai approximation. *Journal of Mathematical Chemistry*, 61(1):47–74, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01408-w`.

Soomro:2023:PBB

[3406] Hira Soomro, Nooraini Zainuddin, Hanita Daud, Joshua Sunday, Noraini Jamaludin, Abdullah Abdullah, Apriyanto Mulono, and Evizal Abdul Kadir. 3-point block backward differentiation formula with an off-step point for the solutions of stiff chemical reaction problems. *Journal of Mathematical Chemistry*, 61(1):75–97, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01402-2`.

Zafar:2023:OEO

[3407] Fiza Zafar, Alicia Cordero, Ifra Ashraf, and Juan R. Torregrosa. An optimal eighth order derivative free multiple root finding numerical method and applications to chemistry. *Journal of Mathematical Chemistry*, 61 (1):98–124, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01411-1`.

Saez:2023:MGM

[3408] S. Sáez. On the modified generalized multidimensional KP equation in plasma physics and fluid dynamics in (3+1) dimensions. *Journal of Mathematical Chemistry*, 61(1):125–143, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01412-0`.

Balasubramanian:2023:OPT

[3409] Krishnan Balasubramanian. Orthogonal polynomials through complex matrix graph theory. *Journal of Mathematical Chemistry*, 61(1):144–

165, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01415-x.

Chen:2023:QAH

[3410] Mengxin Chen and Tian Wang. Qualitative analysis and Hopf bifurcation of a generalized Lengyel–Epstein model. *Journal of Mathematical Chemistry*, 61(1):166–192, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01418-8.

Gonzalez:2023:RDR

[3411] Gerardo Gonzalez, S. A. Alexander, and R. L. Coldwell. Relativistic decay rates of one-electron atoms. *Journal of Mathematical Chemistry*, 61 (1):193–218, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01406-y.

Raghavan:2023:AAH

[3412] Divya Raghavan, J. F. Gómez-Aguilar, and N. Sukavanam. Analytical approach of Hilfer fractional order differential equations using iterative Laplace transform method. *Journal of Mathematical Chemistry*, 61(1): 219–241, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01419-7.

Boyack:2023:BSS

[3413] Rufus Boyack, Asadullah Bhuiyan, Aneca Su, and Frank Marsiglio. The bound-state solutions of the one-dimensional pseudoharmonic oscillator. *Journal of Mathematical Chemistry*, 61(1):242–276, January 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01417-9.

Varga:2023:STP

[3414] Imre Varga. Semiclassical and thermal phase space entropies measuring complexity. *Journal of Mathematical Chemistry*, 61(2):277–287, February 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01355-6.

Aldazabal:2023:SEH

[3415] I. Aldazabal and I. Nagy. Sudden excitations of harmonic normal modes. *Journal of Mathematical Chemistry*, 61(2):288–295, Febru-

ary 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01343-w.

Nagy:2023:PSR

[3416] Á. Nagy. Phase-space Rényi entropy, complexity and thermodynamic picture of density functional theory. *Journal of Mathematical Chemistry*, 61 (2):296–304, February 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01347-6.

Hutcheson:2023:CED

[3417] Anders Hutcheson and Ida-Marie Høyvik. Convergence of the electronic density for a target region in cluster models of a NH_3 molecular crystal. *Journal of Mathematical Chemistry*, 61(2):305–321, February 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01351-w.

Kobayashi:2023:PEG

[3418] Masato Kobayashi, Yuta Oba, Tomoko Akama, and Tetsuya Taketsugu. Practical electronic ground- and excited-state calculation method for lanthanide complexes based on frozen core potential approximation to $4f$ electrons. *Journal of Mathematical Chemistry*, 61(2):322–334, February 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01356-5.

Udvardi:2023:TCF

[3419] László Udvardi and István László. Topological charges of fullerenes. *Journal of Mathematical Chemistry*, 61(2):335–342, February 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01354-7.

Jensen:2023:KEF

[3420] Stig Rune Jensen, Antoine Durdek, Magnar Bjørgve, Peter Wind, Tor Flå, and Luca Frediani. Kinetic energy-free Hartree–Fock equations: an integral formulation. *Journal of Mathematical Chemistry*, 61(2): 343–361, February 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01374-3.

Mate:2023:CMC

[3421] Mihály Máté, Klára Petrov, Szilárd Szalay, and Örs Legeza. Compressing multireference character of wave functions via fermionic mode optimization. *Journal of Mathematical Chemistry*, 61(2):362–375, February 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01379-y`.

Pipek:2023:RMT

[3422] Orsolya Anna Pipek and István Csabai. A revised multi-tissue, multi-platform epigenetic clock model for methylation array data. *Journal of Mathematical Chemistry*, 61(2):376–388, February 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01381-4`.

Qin:2023:APS

[3423] Yupeng Qin, Zhen Wang, and Li Zou. Analytical properties and solutions of a modified Lindemann mechanism with three reaction rate constants. *Journal of Mathematical Chemistry*, 61(3):389–401, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01413-z`.

Frolov:2023:POM

[3424] Alexei M. Frolov. Photodetachment of the outer-most electron(s) in few-electron atomic systems. Variational principle for the cross sections. *Journal of Mathematical Chemistry*, 61(3):402–434, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01410-2`.

Nath:2023:QSI

[3425] Debraj Nath and Ramon Carbó-Dorca. Quantum similarity index and Rényi complexity ratio of Kratzer type potential and compared with that of inverse square and Coulomb type potentials. *Journal of Mathematical Chemistry*, 61(3):435–454, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01414-y`.

Sun:2023:SQC

[3426] Bin Sun, Chia-Liang Lin, and T. E. Simos. Solution to quantum chemistry problems using a phase-fitting, singularly P-stable, cost-effective two-step approach with disappearing phase-lag derivatives

up to order 5. *Journal of Mathematical Chemistry*, 61(3):455–489, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01416-w`.

Gui:2023:AEN

[3427] Tianhao Gui and Hongwei Yang. Application of Euler–Newton homotopy method for azeotrope prediction in vacuum distillation. *Journal of Mathematical Chemistry*, 61(3):490–503, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01420-0`.

Beevers:2023:SAI

[3428] Cameron Beevers, Samantha Francis, and Alberto Roldan. Symmetry analysis of irregular objects. *Journal of Mathematical Chemistry*, 61 (3):504–519, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01423-x`.

Giacomini:2023:CRP

[3429] Josephin Giacomini, Pierluigi Maponi, and Alessia Perticarini. CMMSE: a reduced percolation model for espresso coffee. *Journal of Mathematical Chemistry*, 61(3):520–538, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01428-6`.

Pandit:2023:NAH

[3430] Biswajit Pandit, Mukesh Kumar Rawani, Amit Kumar Verma, and Carlo Cattani. Numerical approximation of higher order singular boundary value problem by using Haar functions. *Journal of Mathematical Chemistry*, 61(3):539–568, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01421-z`.

Belkic:2023:IPR

[3431] Dzevad Belkić and Karen Belkić. Inverse problem for reconstruction of components from derivative envelope in ovarian MRS: Citrate quartet as a cancer biomarker with considerably decreased levels in malignant vs benign samples. *Journal of Mathematical Chemistry*, 61(3): 569–599, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01422-y`.

Bello-Rivas:2023:SCI

[3432] Juan M. Bello-Rivas, Anastasia Georgiou, John Guckenheimer, and Ioannis G. Kevrekidis. Staying the course: iteratively locating equilibria of dynamical systems on Riemannian manifolds defined by point-clouds. *Journal of Mathematical Chemistry*, 61(3):600–629, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01425-9`.

Hernandez:2023:PEP

[3433] Bryan S. Hernandez and Eduardo R. Mendoza. Positive equilibria of power law kinetics on networks with independent linkage classes. *Journal of Mathematical Chemistry*, 61(3):630–651, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01432-w`.

Opoku-Ameyaw:2023:CNT

[3434] Kwaku Opoku-Ameyaw, Celia Nunes, Manuel L. Esquivel, and João T. Mexia. CMMSE: a nonparametric test for grouping factor levels: an application to cocoa breeding experiments in acidic soils. *Journal of Mathematical Chemistry*, 61(3):652–672, March 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01431-x`.

Ramos:2023:NOS

[3435] Higinio Ramos and Mufutau Ajani Rufai. A new one-step method with three intermediate points in a variable step-size mode for stiff differential systems. *Journal of Mathematical Chemistry*, 61(4):673–688, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01427-7`.

Komatsu:2023:SAB

[3436] Hirokazu Komatsu and Hiroshi Yokota. Stability analysis for butlerov chemical reaction in batch reactor. *Journal of Mathematical Chemistry*, 61(4):689–711, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01424-w`.

Flores-Gallegos:2023:ALE

[3437] N. Flores-Gallegos. An approach to local electron energy in atoms through Rényi's entropy. *Journal of Mathematical Chemistry*, 61(4):712–722, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01430-y.

Flores-Gallegos:2023:CBB

[3438] N. Flores-Gallegos. A close-up to the bond-breaking and bond-forming using information theory. *Journal of Mathematical Chemistry*, 61(4): 723–735, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01436-6.

Chicharro:2023:FFO

[3439] Francisco I. Chicharro, Neus Garrido, Julissa H. Jerezano, and Daniel Pérez-Palau. Family of fourth-order optimal classes for solving multiple-root nonlinear equations. *Journal of Mathematical Chemistry*, 61(4): 736–760, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01429-5.

Kaur:2023:EAC

[3440] Anurag Kaur, V. Kanwar, and Higinio Ramos. An efficient algorithm combining an optimized hybrid block method and the differential quadrature method for solving Hunter–Saxton equation. *Journal of Mathematical Chemistry*, 61(4):761–776, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01437-5.

Belkic:2023:HET

[3441] Dzevad Belkić. High-energy two-electron transfer in ion-atom collisions. *Journal of Mathematical Chemistry*, 61(4):777–804, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01426-8. See correction [3442].

Belkic:2023:CHE

[3442] Dzevad Belkić. Correction to: High-energy two-electron transfer in ion-atom collisions. *Journal of Mathematical Chemistry*, 61(4):805, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-022-01445-5. See [3441].

Frezzato:2023:ITC

[3443] Diego Frezzato. Intrinsic timing in classical master equation dynamics from an extended quadratic format of the evolution law. *Journal of*

Mathematical Chemistry, 61(4):806–834, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01435-7`.

Nath:2023:EIE

[3444] Debraj Nath and Amlan K. Roy. Energy and information-entropic measures of Hulthén potential in D dimension by a new approximation to centrifugal term. *Journal of Mathematical Chemistry*, 61(4): 835–858, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01440-w`.

Gurunathan:2023:TCS

[3445] Sambanthan Gurunathan, Thangaraj Yogalakshmi, and Krishnan Balasubramanian. Topological characterization of statistically clustered networks for molecular similarity analysis. *Journal of Mathematical Chemistry*, 61(4):859–876, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01438-4`.

Huang:2023:NWI

[3446] Xin Huang and Li Xia. A novel wavelength interval selection based on split regularized regression for spectroscopic data. *Journal of Mathematical Chemistry*, 61(4):877–892, April 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01444-6`.

Fernandez:2023:CSE

[3447] Francisco M. Fernández. Comment on "Semi-exact solutions of sextic potential plus a centrifugal term". *Journal of Mathematical Chemistry*, 61(5):893–895, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01458-8`. See [3178].

Fortun:2023:CAC

[3448] Noel T. Fortun and Eduardo R. Mendoza. Comparative analysis of carbon cycle models via kinetic representations. *Journal of Mathematical Chemistry*, 61(5):896–932, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01442-8`.

Carballosa:2023:ETI

[3449] Walter Carballosa, Yamilet Quintana, José M. Rodríguez, and José M. Sigarreta. Exponential topological indices: optimal inequalities and

applications. *Journal of Mathematical Chemistry*, 61(5):933–949, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01446-4`.

Manchanda:2023:SSS

[3450] Geetan Manchanda, Gunjan Khurana, and R. K. Mohanty. Superstable spline-in-tension numerical method of order three(four) for the second order nonlinear IVPs. *Journal of Mathematical Chemistry*, 61 (5):950–974, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01441-9`.

Doktorov:2023:DIR

[3451] Alexander B. Doktorov. Diffusion-influenced reactions in the presence of reactivity anisotropy as spots at the poles of a rigid sphere. *Journal of Mathematical Chemistry*, 61(5):975–1003, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01448-w`.

Yamano:2023:IIS

[3452] Takuya Yamano. Inequality-induced similarity measures for radial electronic probability densities in hydrogenic atoms. *Journal of Mathematical Chemistry*, 61(5):1004–1015, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01450-2`.

Carbo-Dorca:2023:QSQ

[3453] Ramon Carbó-Dorca. Quantum similarity and QSPR in Euclidean-, and Minkowskian–Banach spaces. *Journal of Mathematical Chemistry*, 61 (5):1016–1035, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01454-y`.

Wang:2023:TIP

[3454] Yong Wang, Xu Zhou, Weihua Jiang, and Liangping Qi. Turing instability and pattern formation in a diffusive Sel'kov–Schnakenberg system. *Journal of Mathematical Chemistry*, 61(5):1036–1062, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01452-0`.

Eskandari:2023:CBC

[3455] Zohreh Eskandari, R. Khoshsiar Ghaziani, Zakieh Avazzadeh, and Bo Li. Codimension-2 bifurcations on the curve of the Neimark–Sacker bifurcation for a discrete-time chemical model. *Journal of Mathematical Chemistry*, 61(5):1063–1076, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01449-9`.

Fujita:2023:STMa

[3456] Shinsaku Fujita. Stereoisograms for three-membered heterocycles: IV. Half-size-subgroup method for type-itemized enumeration of oxiranes under an *RS*-stereoisomeric group. *Journal of Mathematical Chemistry*, 61 (5):1077–1111, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01434-8`.

Fujita:2023:STMb

[3457] Shinsaku Fujita. Stereoisograms for three-membered heterocycles: V. Factor-group method for type-itemized enumeration of oxiranes under an *RS*-stereoisomeric group. *Journal of Mathematical Chemistry*, 61(5): 1112–1142, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-022-01433-9`.

Poddar:2023:CDI

[3458] Arpita Poddar, Ranita Pal, Chunying Rong, and Pratim Kumar Chattaraj. A conceptual DFT and information-theoretic approach towards QSPR modeling in polychlorobiphenyls. *Journal of Mathematical Chemistry*, 61(5):1143–1164, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01457-9`.

Mohanty:2023:NLC

[3459] R. K. Mohanty and Divya Sharma. A new 2-level compact off-step implicit method in exponential form for the solution of fourth order nonlinear parabolic equations. *Journal of Mathematical Chemistry*, 61(5): 1165–1204, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01451-1`.

Liu:2023:QSA

[3460] Yunmei Liu, Zejie Tian, Hui Li, Zhenhua Liu, Lei Shi, and Lingyan Yang. 3D quantitative structure-activity relationships study on anti-

gastric cancer of chrysin derivatives. *Journal of Mathematical Chemistry*, 61(5):1205–1216, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01455-x`.

Molina:2023:IDI

[3461] Edil D. Molina, José M. Rodríguez, José L. Sánchez, and José M. Sigarreta. Inverse degree index: exponential extension and applications. *Journal of Mathematical Chemistry*, 61(5):1217–1237, May 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01453-z`.

Lam:2023:ECI

[3462] Ching-Wan Lam. Enumeration of constitutional isomers of methyl alkanes by means of alkyl biradicals: equivalence of odd and even isomer series of symmetrical methyl alkanes. *Journal of Mathematical Chemistry*, 61(6):1239–1247, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01469-5`.

Arnrich:2023:NRA

[3463] Steffen Arnrich and Grit Kalies. A natural regularization of the adsorption integral equation with Langmuir-kernel. *Journal of Mathematical Chemistry*, 61(6):1248–1274, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01447-x`.

Jia:2023:CEN

[3464] Ji-Teng Jia and Fu-Rong Wang. A cost-efficient numerical algorithm for the determinants of heptadiagonal matrices with Toeplitz structure. *Journal of Mathematical Chemistry*, 61(6):1275–1291, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01459-7`.

Bracken:2023:MIL

[3465] Paul Bracken. A mathematical investigation of Landauer's principle. *Journal of Mathematical Chemistry*, 61(6):1292–1300, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01463-x`.

Doma:2023:ASM

[3466] S. B. Doma, A. A. Gohar, and M. S. Younes. Analytical solutions of the molecular Kratzer–Feus potential by means of the Nikiforov–Uvarov method. *Journal of Mathematical Chemistry*, 61(6):1301–1312, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01462-y`.

Singh:2023:RNT

[3467] Satpal Singh, Devendra Kumar, and J. Vigo-Aguiar. A robust numerical technique for weakly coupled system of parabolic singularly perturbed reaction-diffusion equations. *Journal of Mathematical Chemistry*, 61(6):1313–1350, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01464-w`.

Fujita:2023:STMc

[3468] Shinsaku Fujita. Stereoisograms for three-membered heterocycles: V. factor-group method for type-itemized enumeration of oxiranes under an *RS*-stereoisomeric group. *Journal of Mathematical Chemistry*, 61(6):1351–1382, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01456-w`.

Nath:2023:ITS

[3469] Debraj Nath and Ramon Carbó-Dorca. Information-theoretic spreading measures of a particle confined in a 3D infinite spherical well. *Journal of Mathematical Chemistry*, 61(6):1383–1402, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01460-0`.

Yildiz:2023:SAA

[3470] Burhan Yildiz, Cem Kaanoglu, and Vali Bashiry. Shape analysis of an axisymmetric pendant drop using minimization of free energy. *Journal of Mathematical Chemistry*, 61(6):1403–1413, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01468-6`.

Lin:2023:PFS

[3471] Chia-Liang Lin and T. E. Simos. Phase-fitting, singularly *P*-stable, cost-effective two-step approach to solving problems in quantum chemistry with vanishing phase-lag derivatives up to order 6. *Journal of Mathematical Chemistry*, 61(6):1414–1452, July 2023. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01461-z`.

Flores-Gallegos:2023:FDE

[3472] N. Flores-Gallegos. Fermi–Dirac entropy as a measure of electron interactions. *Journal of Mathematical Chemistry*, 61(6):1453–1461, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01466-8`.

Popat:2023:SNR

[3473] Kalpesh M. Popat and Kunal R. Shingala. Some new results on energy of graphs with self loops. *Journal of Mathematical Chemistry*, 61(6): 1462–1469, July 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01467-7`.

Balasubramanian:2023:RAP

[3474] Krishnan Balasubramanian and Ernest R. Davidson. Rational approximations to pie: transcendental π and Euler's constant e. *Journal of Mathematical Chemistry*, 61(7):1471–1476, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01480-w`.

Govardhan:2023:TIE

[3475] S. Govardhan, S. Roy, Krishnan Balasubramanian, and S. Prabhu. Topological indices and entropies of triangular and rhomboidal tessellations of kekulenes with applications to NMR and ESR spectroscopies. *Journal of Mathematical Chemistry*, 61(7):1477–1490, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01465-9`.

Nath:2023:AES

[3476] Debraj Nath and Amlan K. Roy. Average energy and Shannon entropy of a confined harmonic oscillator in a time-dependent moving boundary. *Journal of Mathematical Chemistry*, 61(7):1491–1503, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01471-x`.

Jia:2023:EAD

[3477] Ji-Teng Jia and Fu-Rong Wang. On the efficient and accurate determinant evaluation of periodic tridiagonal Toeplitz matrices. *Journal of*

Mathematical Chemistry, 61(7):1504–1521, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01474-8`.

Mao:2023:SAC

[3478] Guoyong Mao, Runzhan Liu, and Ning Zhang. Similarity analysis of chemical elements based on compounds network. *Journal of Mathematical Chemistry*, 61(7):1522–1531, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01473-9`.

Flores-Gallegos:2023:IOU

[3479] N. Flores-Gallegos. On the information obtained using Shannon's entropy through spin density. *Journal of Mathematical Chemistry*, 61(7):1532–1544, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01481-9`.

Lin:2023:HES

[3480] Chia-Liang Lin and T. E. Simos. Highly efficient, singularly p-stable, and low-cost phase-fitting two-step method of 14th order for problems in chemistry. *Journal of Mathematical Chemistry*, 61(7):1545–1569, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01470-y`.

Balasubramanian:2023:CPS

[3481] Krishnan Balasubramanian. Characteristic polynomials, spectral-based Riemann-zeta functions and entropy indices of n-dimensional hypercubes. *Journal of Mathematical Chemistry*, 61(7):1570–1591, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01479-3`.

Klavzar:2023:CMH

[3482] Sandi Klavzar and Gasper Domen Romih. The cut method on hypergraphs for the Wiener index. *Journal of Mathematical Chemistry*, 61(7):1592–1603, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01478-4`.

Dlamini:2023:SSB

[3483] Phumlani Dlamini, James Malele, and Simphiwe Simelane. Solving singular boundary value problems using higher-order compact finite dif-

ference schemes with a novel higher-order implementation of Robin boundary conditions. *Journal of Mathematical Chemistry*, 61(7):1604–1632, August 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01475-7`.

Arockiaraj:2023:COF

[3484] Micheal Arockiaraj, Joseph Jency, Shagufa Mushtaq, Arul Jeya Shalini, and Krishnan Balasubramanian. Covalent organic frameworks: topological characterizations, spectral patterns and graph entropies. *Journal of Mathematical Chemistry*, 61(8):1633–1664, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01477-5`.

Morales-Bayuelo:2023:PWQ

[3485] Alejandro Morales-Bayuelo. A possible way to quantify the *philicity* using molecular quantum similarity and chemical reactivity indices. *Journal of Mathematical Chemistry*, 61(8):1665–1671, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01482-8`.

Coskun:2023:ANB

[3486] M. Coskun and M. Ertürk. Applicability of noninteger Bessel type orbital basis sets: numerical and analytical approaches. *Journal of Mathematical Chemistry*, 61(8):1672–1683, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01484-6`.

Dong:2023:ESS

[3487] Shi-Hai Dong and Guo-Hua Sun. Exact solutions of the Schrödinger equation with a complex periodic potential. *Journal of Mathematical Chemistry*, 61(8):1684–1695, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01483-7`.

Paul:2023:AEF

[3488] Jayanta Paul, Debdulal Ghosh, and Jitendra Kumar. Accurate and efficient flux-corrected finite volume approximation for the fragmentation problem. *Journal of Mathematical Chemistry*, 61(8):1696–1716, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01485-5`.

Chattaraj:2023:MCC

[3489] Pratim Kumar Chattaraj and Ranita Pal. A modified cusp condition for the single density equations of DFT and orbital-free DFT for atoms. *Journal of Mathematical Chemistry*, 61(8):1717–1725, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01487-3`.

Flores-Gallegos:2023:ACH

[3490] N. Flores-Gallegos and L. Flores-Gómez. An approach to chemical hardness through Shannon's entropy. *Journal of Mathematical Chemistry*, 61(8):1726–1738, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01488-2`.

Vivas-Reyes:2023:GDI

[3491] Ricardo Vivas-Reyes, Oscar Martínez-Santiago, and Yovani Marrero-Ponce. Graph derivative indices interpretation from the quantum mechanics perspective. *Journal of Mathematical Chemistry*, 61(8):1739–1757, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01489-1`.

Zhuk:2023:TDT

[3492] P. F. Zhuk and S. O. Karakhim. Two different types of kinetics, where the initial rate increases faster or slower than the reactant concentration, can coexist on bell-shaped kinetic dependencies. *Journal of Mathematical Chemistry*, 61(8):1758–1796, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01491-7`.

Bao:2023:TSF

[3493] Wei Bao, Chia-Liang Lin, Bin Sun, and T. E. Simos. Two-step, fourteenth-order, phase-fitting procedure with high efficiency and minimal cost for chemical problems. *Journal of Mathematical Chemistry*, 61(8):1797–1823, September 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01486-4`.

Jha:2023:TUM

[3494] Ruchi Jha, Shanti Gopal Patra, Himangshu Mondal, and Pratim Kumar Chattaraj. Theoretical understanding of mechanochemical (ball-milling) synthesis of thioethers: a CDFT approach. *Journal of Mathe-*

matical Chemistry, 61(9):1825–1841, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01492-6`.

Roul:2023:OCM

[3495] Pradip Roul, V. M. K. Prasad Goura, and Ravi Agarwal. An optimal computational method for a general class of nonlinear boundary value problems. *Journal of Mathematical Chemistry*, 61(9):1842–1878, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01493-5`.

Fernandez:2023:EBG

[3496] Francisco M. Fernández. Extremely broken generalized $\mathcal{PT}$ symmetry. *Journal of Mathematical Chemistry*, 61(9):1879–1887, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01496-2`.

Medvedeva:2023:SQC

[3497] Marina A. Medvedeva and T. E. Simos. Solution of quantum chemical problems by a very effective and relatively inexpensive two-step, fourteenth-order, phase-fitting procedure. *Journal of Mathematical Chemistry*, 61(9):1888–1915, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01490-8`.

Carbo-Dorca:2023:SFC

[3498] Ramon Carbó-Dorca and Debraj Nath. A study of Fermionic Cooper pairs. *Journal of Mathematical Chemistry*, 61(9):1916–1923, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01499-z`.

Kumari:2023:AFS

[3499] Dimple Kumari, Saloni Saloni, Martín Labarca, and Tanmoy Chakraborty. Application of Floating Spherical Gaussian Orbital approach in redefining the atomic periodic descriptor. *Journal of Mathematical Chemistry*, 61(9):1924–1935, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01494-4`.

Belkic:2023:DSE

[3500] Dzevad Belkić and Karen Belkić. Derivative shape estimations with resolved overlapped peaks and reduced noise for time signals encoded by NMR spectroscopy with and without water suppression. *Journal of Mathematical Chemistry*, 61(9):1936–1966, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01500-9`.

Arteca:2023:ICE

[3501] Gustavo A. Arteca. Interpretation of covolume in an extension of the Redlich–Kwong equation of state for real gases. *Journal of Mathematical Chemistry*, 61(9):1967–1979, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01497-1`.

Plesa:2023:IFS

[3502] Tomislav Plesa, Alexander Dack, and Thomas E. Ouldridge. Integral feedback in synthetic biology: negative-equilibrium catastrophe. *Journal of Mathematical Chemistry*, 61(9):1980–2018, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01495-3`.

Belkic:2023:VMD

[3503] Dzevad Belkić. Various mechanisms for double capture from helium targets by alpha particles. *Journal of Mathematical Chemistry*, 61(9):2019–2044, October 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01502-7`.

Du:2023:SQC

[3504] Yu Du, Chia-Liang Lin, Bin Sun, and T. E. Simos. Solution of quantum chemical problems using an extremely successful and reasonably cost two-step, fourteenth-order phase-fitting approach. *Journal of Mathematical Chemistry*, 61(10):2045–2078, November 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01498-0`.

Singh:2023:MMD

[3505] Malkesh Singh, Sunny Kumar Sharma, and Vijay Kumar Bhat. On mixed metric dimension of crystal cubic carbon structure. *Journal of Mathematical Chemistry*, 61(10):2079–2097, November 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01507-2`.

Srivastava:2023:TPT

[3506] Shivam Srivastava, Anjani K. Pandey, and Chandra K. Dixit. Theoretical prediction for thermoelastic properties of carbon nanotubes (CNTs) at different pressure or compression using equation of states. *Journal of Mathematical Chemistry*, 61(10):2098–2104, November 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01506-3`.

Hernandez:2023:NBP

[3507] Bryan S. Hernandez and Kaitlyn Deen E. Buendicho. A network-based parametrization of positive steady states of power-law kinetic systems. *Journal of Mathematical Chemistry*, 61(10):2105–2122, November 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01505-4`.

Mohanty:2023:TFO

[3508] R. K. Mohanty. Third (fourth) order accurate two-step super-stable cubic spline polynomial approximation for the second order non-linear initial-value problems. *Journal of Mathematical Chemistry*, 61(10):2123–2145, November 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01509-0`.

Roul:2023:HOC

[3509] Pradip Roul, V. M. K. Prasad Goura, and Ravi Agarwal. A high-order compact finite difference scheme and its analysis for the time-fractional diffusion equation. *Journal of Mathematical Chemistry*, 61(10):2146–2175, November 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01510-7`.

Yadav:2023:GCD

[3510] Sonia Yadav and Sukhjit Singh. Global convergence domains for an efficient fifth order iterative scheme. *Journal of Mathematical Chemistry*, 61(10):2176–2191, November 2023. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01514-3`.

Surjan:2024:ESI

[3511] Péter Surján and Ágnes Szabados. Editorial to the special issue of the *Journal of Mathematical Chemistry* "In Memoriam János Pipek". *Jour-*

nal of Mathematical Chemistry, 62(1):1–2, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01515-2`.

Molski:2024:IEF

[3512] Marcin Molski. Improved energy formula for highly excited vibrational states of Kratzer–Fues oscillator. *Journal of Mathematical Chemistry*, 62(1):3–23, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01513-4`.

Manohara:2024:NSS

[3513] G. Manohara and S. Kumbinarasaiah. Numerical solution of some stiff systems arising in chemistry via Taylor wavelet collocation method. *Journal of Mathematical Chemistry*, 62(1):24–61, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01508-1`.

Flores-Gallegos:2024:ATE

[3514] N. Flores-Gallegos and Alejandro Morales-Bayuelo. An analysis of the torquoselectivity effect in a ring-opening reaction through Fermi–Dirac's entropy: revealing the origin of the stereoselectivity. *Journal of Mathematical Chemistry*, 62(1):62–72, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01519-y`.

Lal:2024:TIG

[3515] Sohan Lal, Vijay Kumar Bhat, and Sahil Sharma. Topological indices and graph entropies for carbon nanotube Y-junctions. *Journal of Mathematical Chemistry*, 62(1):73–108, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01520-5`.

Kansal:2024:ASL

[3516] Munish Kansal and Litika Rani. An adaptive Steffensen-like families for solving nonlinear systems using frozen divided differences. *Journal of Mathematical Chemistry*, 62(1):109–144, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01524-1`.

Choudhary:2024:CBN

[3517] Renu Choudhary and Devendra Kumar. Collocation-based numerical simulation of fractional order Allen–Cahn equation. *Journal of Math-*

ematical Chemistry, 62(1):145–168, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01525-0`.

Sun:2024:HBP

[3518] Yihuan Sun and Shanshan Chen. Hopf bifurcation and periodic solutions in a coupled Brusselator model of chemical reactions. *Journal of Mathematical Chemistry*, 62(1):169–197, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01528-x`.

Kansal:2024:AOI

[3519] Munish Kansal and Himani Sharma. Analysis of optimal iterative methods from a dynamical point of view by studying their stability properties. *Journal of Mathematical Chemistry*, 62(1):198–221, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01523-2`.

Cassam-Chenai:2024:CAG

[3520] Patrick Cassam-Chenaï. A conjecture on antisymmetrized geminal power wavefunctions. *Journal of Mathematical Chemistry*, 62(1):222–227, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01522-3`.

Molina:2024:AID

[3521] Edil D. Molina, José M. Rodríguez, José L. Sánchez, and José M. Sigarreta. Applications of the inverse degree index to molecular structures. *Journal of Mathematical Chemistry*, 62(1):228–249, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01526-z`.

Mendez-Bermudez:2024:VIS

[3522] J. A. Méndez-Bermúdez, Rosalio Reyes, José M. Sigarreta, and María Villeta. On the variable inverse sum deg index: theory and applications. *Journal of Mathematical Chemistry*, 62(1):250–268, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01529-w`.

Pandey:2024:TMP

[3523] Anjani K. Pandey, Chandra K. Dixit, and Shivam Srivastava. Theoretical model for the prediction of lattice energy of diatomic metal halides. *Journal of Mathematical Chemistry*, 62(1):269–274, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01538-9`.

Morales:2024:GAA

[3524] Juan C. Morales and Carlos A. Arango. Geometric-algebraic approach to aqueous solutions of diprotic acids and its buffer mixtures. *Journal of Mathematical Chemistry*, 62(1):275–299, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01527-y`.

Flores-Gallegos:2024:AHP

[3525] N. Flores-Gallegos and O. G-Damián. An approach to Hammond's principle through Kullback–Leibler's entropy. *Journal of Mathematical Chemistry*, 62(1):300–311, January 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01534-z`.

Fernandez:2024:POM

[3526] Francisco M. Fernández. On the pseudoharmonic oscillator as a model for the electronic potential-energy function of a diatomic molecule. *Journal of Mathematical Chemistry*, 62(2):313–316, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01530-3`.

Raychaudhury:2024:IPO

[3527] Chandan Raychaudhury, Shreyaa Srinivasan, and Debnath Pal. Identification of potential oral cancer drugs as Bcl-2 inhibitors from known anti-neoplastic agents through docking studies. *Journal of Mathematical Chemistry*, 62(2):317–329, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01537-w`.

Liu:2024:HOS

[3528] Changying Liu, Yumeng Tang, Jiashang Yu, and Yonglei Fang. High-order symmetric and energy-preserving collocation integrators for the second-order Hamiltonian system. *Journal of Mathematical Chemistry*, 62(2):330–355, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01536-x`.

Gao:2024:UCE

[3529] Ziyao Gao, Jianfeng He, Jing Li, and Kingsley Leung. Unraveling the complexity of Exendin-4 folding through two distinct pathways. *Journal of Mathematical Chemistry*, 62(2):356–366, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01535-y`.

Donati:2024:AAC

[3530] Luca Donati, Konstantin Fackeldey, and Marcus Weber. Augmented ant colony algorithm for virtual drug discovery. *Journal of Mathematical Chemistry*, 62(2):367–385, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01549-6`.

Craciun:2024:CDT

[3531] Gheorghe Craciun, Abhishek Deshpande, and Jiaxin Jin. On the connectivity of the disguised toric locus of a reaction network. *Journal of Mathematical Chemistry*, 62(2):386–405, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01533-0`.

Celebre:2024:MMS

[3532] Giorgio Celebre. Might molecular symmetry operations exist "partially"? *Journal of Mathematical Chemistry*, 62(2):406–424, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01541-0`.

Rajaraman:2024:WBM

[3533] R. Rajaraman. Wavelet-based mathematical analysis of immobilized enzymes in porous catalysts under nonlinear Michaelis–Menten kinetics. *Journal of Mathematical Chemistry*, 62(2):425–460, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01548-7`.

Martinez-Araya:2024:WLH

[3534] Jorge I. Martínez-Araya. Why are the local hyper-softness and the local softness more appropriate local reactivity descriptors than the dual descriptor and the Fukui function, respectively? *Journal of Mathematical Chemistry*, 62(2):461–475, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://`

link.springer.com/article/10.1007/s10910-023-01539-8. See corrections [3581, 3591, 3620].

Craciun:2024:WRS

[3535] Gheorghe Craciun, Abhishek Deshpande, and Jiaxin Jin. Weakly reversible single linkage class realizations of polynomial dynamical systems: an algorithmic perspective. *Journal of Mathematical Chemistry*, 62(2): 476–501, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01540-1.

Doktorov:2024:GRB

[3536] Alexander B. Doktorov and Nikita N. Lukzen. General relationships between the kinetic characteristics of bulk and geminate recombination of radicals in solutions. *Journal of Mathematical Chemistry*, 62(2): 502–521, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01550-z.

Srivastava:2024:CSE

[3537] Shivam Srivastava, Anjani K. Pandey, and Chandra K. Dixit. Comparative study of elastic properties of some inorganic and organic molecular crystals from EOS. *Journal of Mathematical Chemistry*, 62(2): 522–533, February 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01546-9.

Belkic:2024:ODF

[3538] Dzevad Belkić and Karen Belkić. Optimized derivative fast Fourier transform with high resolution and low noise from encoded time signals: Ovarian NMR spectroscopy. *Journal of Mathematical Chemistry*, 62(3):535–554, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01553-w.

Lin:2024:HRB

[3539] Hao Lin, Yiwei Shi, and Shuyang Dai. Hybrid random batch idea and nonlinear conjugate gradient method for accelerating charged polymer dynamics simulation. *Journal of Mathematical Chemistry*, 62(3): 555–578, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01547-8.

Alshammari:2024:TEC

[3540] Nawa A. Alshammari. Two energies for conjoining boron nitride nanotorus and nanotube. *Journal of Mathematical Chemistry*, 62(3):579–590, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01551-y`.

Morales-Bayuelo:2024:QDS

[3541] Alejandro Morales-Bayuelo. Quantifying the distortion by spin-orbit and spin-spin coupling in molecular clusters using molecular quantum similarity. *Journal of Mathematical Chemistry*, 62(3):591–605, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01552-x`.

Belkic:2024:QMF

[3542] Dzevad Belkić. Quantum-mechanical four-body versus semi-classical three-body theories for double charge exchange in collisions of fast alpha particles with helium targets. *Journal of Mathematical Chemistry*, 62 (3):606–633, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01564-7`.

Celik:2024:EMD

[3543] Esra Celik, Huseyin Tunc, and Murat Sari. An efficient multi-derivative numerical method for chemical boundary value problems. *Journal of Mathematical Chemistry*, 62(3):634–653, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01556-7`.

Gozukirmizi:2024:PQS

[3544] Cosar Gözükirmizi. Pure quadratization and solution of ordinary differential equations by probabilistic evolution theory with concurrent computation of coefficients using exact arithmetic. *Journal of Mathematical Chemistry*, 62(3):654–680, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01563-8`.

Reed:2024:AAN

[3545] B. Cameron Reed and Gregory L. Bason. An alternative approach to normalizing the Coulomb $R_{n\ell}(r)$ radial solutions. *Journal of Mathematical Chemistry*, 62(3):681–688, March 2024. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01562-9.

Vigo-Aguiar:2024:IST

[3546] J. Vigo-Aguiar, Reetika Chawla, Devendra Kumar, and Tapas Mazumdar. An implicit scheme for time-fractional coupled generalized Burgers' equation. *Journal of Mathematical Chemistry*, 62(3):689–710, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01559-4.

Melgaard:2024:SAS

[3547] M. Melgaard and V. J. J. Syrjanen. Spectral approximation scheme for a hybrid, spin-density Kohn–Sham density-functional theory in an external (nonuniform) magnetic field and a collinear exchange-correlation energy. *Journal of Mathematical Chemistry*, 62(3):711–760, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01557-6.

Medvedeva:2024:EEI

[3548] Marina A. Medvedeva and T. E. Simos. An exceedingly effective and inexpensive two-step, fourteenth-order phase-fitting method for solving quantum chemical issues. *Journal of Mathematical Chemistry*, 62(3):761–801, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01560-x.

Chavez:2024:IPB

[3549] Andy A. Chavez, Alec P. Adam, Paul W. Ayers, and Ramón Alain Miranda-Quintana. Inductive proof of Borchardt's theorem. *Journal of Mathematical Chemistry*, 62(3):802–808, March 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01561-w.

Raja:2024:TES

[3550] Nadar Jenita Mary Masilamani Raja and A. Anuradha. Topological entropies of single walled carbon nanotubes. *Journal of Mathematical Chemistry*, 62(4):809–818, April 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01532-1.

Sabirov:2024:HLR

[3551] Denis Sh. Sabirov, Alexandra D. Zimina, and Alina A. Tukhbatullina. Hess' law requires modified mathematical rules for information entropy of interdependent chemical reactions. *Journal of Mathematical Chemistry*, 62(4):819–835, April 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01566-5`.

Sakariya:2024:NST

[3552] Harshad Sakariya and Sushil Kumar. Numerical simulation of the time fractional Gray–Scott model on 2D space domains using radial basis functions. *Journal of Mathematical Chemistry*, 62(4):836–864, April 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01571-8`.

Ghosh:2024:LPC

[3553] Paulami Ghosh and Nabakumar Bera. Laws of physical chemistry: a potential tool for generating some series and to evaluate their sum. *Journal of Mathematical Chemistry*, 62(4):865–886, April 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01572-7`.

Vyshnavi:2024:GTN

[3554] D. Vyshnavi and B. Chaluvaraju. Generalized transmission neighbor indices: graph connectivity analysis and its chemical relevance. *Journal of Mathematical Chemistry*, 62(4):887–901, April 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01567-4`.

Sajjad:2024:CRD

[3555] Wasim Sajjad, Xiang-Feng Pan, and Qura tul Ain. Computation of resistance distance with Kirchhoff index of body centered cubic structure. *Journal of Mathematical Chemistry*, 62(4):902–921, April 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01573-6`.

Ventura:2024:KTC

[3556] E. Ventura, Rodolpho L. R. Alves, and Silmar A. do Monte. The kinetics of three coupled irreversible elementary reactions: two parallel mixed second order reactions followed by a first order reaction. *Journal of Mathematical Chemistry*, 62(4):922–935, April 2024. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01580-1.

Dias:2024:INP

[3557] Jerry Ray Dias. Isomer number patterns in aromatic hydrocarbon chemistry: the numbers speak for themselves. *Journal of Mathematical Chemistry*, 62(5):937–950, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01579-8.

Barabas:2024:PVB

[3558] Béla Barabás, Ottilia Fülöp, Marcell Nagy, and Gyula Pályi. Progress in the valorization of biomass: a statistical perspective. *Journal of Mathematical Chemistry*, 62(5):951–972, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01575-y.

Mohanty:2024:NLI

[3559] R. K. Mohanty and Divya Sharma. A new 2-level implicit high accuracy compact exponential approximation for the numerical solution of nonlinear fourth order Kuramoto–Sivashinsky and Fisher–Kolmogorov equations. *Journal of Mathematical Chemistry*, 62(5): 973–1011, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01577-w.

Gagrani:2024:PGC

[3560] Praful Gagrani, Victor Blanco, Eric Smith, and David Baum. Polyhedral geometry and combinatorics of an autocatalytic ecosystem. *Journal of Mathematical Chemistry*, 62(5):1012–1078, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01576-x.

Alizadeh:2024:SMI

[3561] Yaser Alizadeh, Nino Bašić, Ivan Damnjanović, Tomislav Došlić, Tomaž Pisanski, Dragan Stevanović, and Kexiang Xu. Solving the Mostar index inverse problem. *Journal of Mathematical Chemistry*, 62(5): 1079–1093, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01581-0.

Martinez-Araya:2024:DDP

[3562] Jorge I. Martínez-Araya. The dual descriptor potential. *Journal of Mathematical Chemistry*, 62(5):1094–1112, May 2024. CODEN JM-

CHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01583-y`. See corrections [3563, 3605, 3605].

Martinez-Araya:2024:CDDa

[3563] Jorge Martínez-Araya. Correction: The dual descriptor potential. *Journal of Mathematical Chemistry*, 62(5):1113, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01616-6`. See [3562, 3605].

Eghbaljoo:2024:ASD

[3564] Mozhgan Eghbaljoo, Gholamreza Hojjati, and Ali Abdi. Adaptive second derivative multistep methods for solving stiff chemical problems. *Journal of Mathematical Chemistry*, 62(5):1114–1133, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01582-z`.

Bose:2024:EAS

[3565] Sonu Bose and Kaushik Mukherjee. Efficient approximation of solution derivatives for system of singularly perturbed time-dependent convection-diffusion PDEs on Shishkin mesh. *Journal of Mathematical Chemistry*, 62(5):1134–1174, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01587-8`.

Molski:2024:IRK

[3566] Marcin Molski. Improved rotating Kratzer–Fues oscillator: eigenenergies, eigenfunctions, coherent states and ladder operators. *Journal of Mathematical Chemistry*, 62(5):1175–1188, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01585-w`.

Jeon:2024:NAT

[3567] Yonghyeon Jeon and Sunyoung Bu. Numerical approach for time-fractional Burgers' equation via a combination of Adams–Moulton and linearized technique. *Journal of Mathematical Chemistry*, 62(5):1189–1208, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01589-6`.

Yuan:2024:TPP

[3568] Pingfang Yuan, Zhenfeng Liu, Yanxin Xie, Yafei Meng, Mengdie Li, and Keke Chen. On the thermal properties of pure and defective Ψ-graphene nanotubes by molecular dynamics simulations. *Journal of Mathematical Chemistry*, 62(5):1209–1221, May 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01588-7`.

Saadat:2024:FPF

[3569] Hosein Saadat, Sanaz Hami Hassan Kiyadeh, Ramin Goudarzi Karim, and Ali Safaie. Family of phase fitted 3-step second-order BDF methods for solving periodic and orbital quantum chemistry problems. *Journal of Mathematical Chemistry*, 62(6):1223–1250, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01619-3`.

Belkic:2024:VBM

[3570] Dzevad Belkić and Karen Belkić. In vivo brain MRS at a 1.5T clinical scanner: Optimized derivative fast Fourier transform for high-resolution spectra from time signals encoded with and without water suppression. *Journal of Mathematical Chemistry*, 62(6):1251–1286, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01597-6`.

Vinod:2024:UTD

[3571] Y. Vinod, Suma Nagendrappa Nagappanavar, Sangamesh, K. R. Raghunatha, and D. L. Kiran Kumar. Unsteady triple diffusive oscillatory flow in a Voigt fluid. *Journal of Mathematical Chemistry*, 62(6):1287–1307, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01591-y`.

Roul:2024:HOB

[3572] Pradip Roul. A high-order B-spline collocation method for solving a class of nonlinear singular boundary value problems. *Journal of Mathematical Chemistry*, 62(6):1308–1322, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01590-z`.

Shi:2024:TTG

[3573] Yang Shi and Xuehua Yang. A time two-grid difference method for nonlinear generalized viscous Burgers' equation. *Journal of Mathematical*

Chemistry, 62(6):1323–1356, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01592-x`.

Garcia-Chung:2024:CIE

[3574] Angel Garcia-Chung, Marisol Bermúdez-Montaña, Peter F. Stadler, Jürgen Jost, and Guillermo Restrepo. Chemically inspired Erdős–Rényi hypergraphs. *Journal of Mathematical Chemistry*, 62(6):1357–1383, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01595-8`.

Cen:2024:IDS

[3575] Zhongdi Cen, Jian Huang, and Aimin Xu. An integral discretization scheme on a graded mesh for a fractional differential equation with integral boundary conditions. *Journal of Mathematical Chemistry*, 62(6):1384–1398, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01596-7`.

Belkic:2024:CSS

[3576] Dzevad Belkić. Cross section sensitivity to perturbation strengths in distorted waves for double electron capture by alpha particles from helium targets. *Journal of Mathematical Chemistry*, 62(6):1399–1423, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01599-4`.

BenTorkia:2024:RBL

[3577] Yosra Ben Torkia and Abdelmottaleb Ben Lamine. Relationship between Lennard-Jones potential and physico-chemical parameters. *Journal of Mathematical Chemistry*, 62(6):1424–1434, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01598-5`.

Granados:2024:NBV

[3578] Ana Granados, Ana Portilla, Yamilet Quintana, and Eva Tourís. New bounds for variable topological indices and applications. *Journal of Mathematical Chemistry*, 62(6):1435–1453, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01593-w`.

Kothari:2024:ESE

[3579] Samay Kothari and Abhishek Deshpande. Endotactic and strongly endotactic networks with infinitely many positive steady states. *Journal of Mathematical Chemistry*, 62(6):1454–1478, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01617-5`.

Herbig:2024:PCC

[3580] Hans-Christian Herbig. Pivotal condensation and chemical balancing. *Journal of Mathematical Chemistry*, 62(6):1479–1519, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01594-9`.

Martinez-Araya:2024:CWLa

[3581] Jorge I. Martínez-Araya. Correction: Why are the local hyper-softness and the local softness more appropriate local reactivity descriptors than the dual descriptor and the Fukui function, respectively? *Journal of Mathematical Chemistry*, 62(6):1520, July 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01613-9`. See [3534].

Aghili:2024:ESR

[3582] Alireza Aghili and Amir Hossein Shabani. Evaluation of smooth reaction rate of noisy experimental data using Legendre series expansion. *Journal of Mathematical Chemistry*, 62(7):1521–1536, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01618-4`.

Colquhoun:2024:NRT

[3583] Howard M. Colquhoun and Ricardo Grau-Crespo. Numerical representations of AB-type copolymer complexes: analysis of ^{1}H NMR chemical shift patterns in terms of a Smith–Cantor set. *Journal of Mathematical Chemistry*, 62(7):1537–1557, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01614-8`.

Singh:2024:IVF

[3584] Manpal Singh, S. Das, and Rajeev. An innovative Vieta–Fibonacci wavelet collocation method for the numerical solution of three-component Brusselator reaction diffusion system of fractional order. *Journal of*

Mathematical Chemistry, 62(7):1558–1594, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01621-9`.

Doslic:2024:FCR

[3585] Tomislav Doslić. Fusene chains revisited: how kinky they are and why it matters. *Journal of Mathematical Chemistry*, 62(7):1595–1606, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01620-w`.

Medvedeva:2024:LCT

[3586] Marina A. Medvedeva and T. E. Simos. A low-cost, two-step fourteenth-order phase-fitting approach to tackling problems in chemistry. *Journal of Mathematical Chemistry*, 62(7):1607–1646, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01615-7`.

Alamin:2024:PSS

[3587] Al Jay Lan J. Alamin and Bryan S. Hernandez. Positive steady states of a class of power law systems with independent decompositions. *Journal of Mathematical Chemistry*, 62(7):1647–1666, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01622-8`.

Liu:2024:NTE

[3588] Kai Liu, Ting Fu, Wei Shi, and Xuhuan Zhou. A new type of energy-preserving integrators for quasi-bi-Hamiltonian systems. *Journal of Mathematical Chemistry*, 62(7):1667–1681, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01624-6`.

Dutt:2024:AED

[3589] A. K. Dutt. Amplitude equation for a diffusion–reaction system in presence of complexing reaction with the activator species: the Brusselator model. *Journal of Mathematical Chemistry*, 62(7):1682–1726, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01574-z`.

Das:2024:CDR

[3590] Sanatan Das, Poly Karmakar, Tilak Kumar Pal, Soumitra Sarkar, Asgar Ali, and Rabindra Nath Jana. Chemical dynamics in a radioac-

tive platinum–cerium oxide–water mixture within a vibrating Riga channel subject to sudden pressure gradient onset. *Journal of Mathematical Chemistry*, 62(7):1727–1778, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01625-5`.

Martinez-Araya:2024:CWLb

[3591] Jorge I. Martínez-Araya. Correction: Why local softness and local hypersoftness are more appropriate local reactivity descriptors than dual descriptor and Fukui functions? *Journal of Mathematical Chemistry*, 62 (7):1779, August 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01629-1`. See [3534].

Xu:2024:UMC

[3592] Rong Xu, Bin Sun, Chia-Liang Lin, and T. E. Simos. The use of a multistep, cost-efficient fourteenth-order phase-fitting method to chemistry problems. *Journal of Mathematical Chemistry*, 62(8):1781–1807, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01623-7`.

Jia:2024:ENA

[3593] Ji-Teng Jia, Fu-Rong Wang, Rong Xie, and Yi-Fan Wang. An efficient numerical algorithm for solving linear systems with cyclic tridiagonal coefficient matrices. *Journal of Mathematical Chemistry*, 62(8):1808–1821, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01631-7`.

Kabeto:2024:ECM

[3594] Masho Jima Kabeto, Tesfaye Aga Bullo, Habtamu Garoma Debela, Gemadi Roba Kusi, and Sisay Dibaba Robi. Efficient computational method for singularly perturbed Burger–Huxley equations. *Journal of Mathematical Chemistry*, 62(8):1822–1833, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01627-3`.

Rao:2024:AAS

[3595] S. Chandra Sekhara Rao and Varsha Srivastava. Analysis of an almost second-order parameter-robust numerical technique for a weakly coupled system of singularly perturbed convection-diffusion equations. *Journal of Mathematical Chemistry*, 62(8):1834–1859, September 2024. CODEN

JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01634-4.

Huang:2024:EMF

[3596] Hui Huang, Cheng Liu, Chia-Liang Lin, and T. E. Simos. An effective multistep fourteenth-order phase-fitting approach to solving chemistry problems. *Journal of Mathematical Chemistry*, 62(8):1860–1889, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01628-2.

Zhang:2024:DBC

[3597] Xiaofeng Zhang and Shulin Sun. Dynamical behavior of a classical stochastic delayed chemostat model. *Journal of Mathematical Chemistry*, 62(8):1890–1911, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01632-6.

Chawla:2024:NIT

[3598] Reetika Chawla, Devendra Kumar, and Dumitru Baleanu. Numerical investigation of two fractional operators for time fractional delay differential equation. *Journal of Mathematical Chemistry*, 62(8):1912–1934, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01637-1.

Bernhoff:2024:LBC

[3599] Niclas Bernhoff. Linearized Boltzmann collision operator for a mixture of monatomic and polyatomic chemically reacting species. *Journal of Mathematical Chemistry*, 62(8):1935–1964, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01633-5.

Wawrzyniak:2024:GRS

[3600] Piotr Wawrzyniak and Piotr Formanowicz. Graph realization of sets of integers. *Journal of Mathematical Chemistry*, 62(8):1965–1981, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01642-4.

Kumari:2024:PUH

[3601] Parvin Kumari, Devendra Kumar, and Jesus Vigo-Aguiar. A parameter-uniform hybrid scheme designed for multi-point boundary value problems

that are perturbed. *Journal of Mathematical Chemistry*, 62(8):1982–2006, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01639-z`.

Bhavna:2024:CAO

[3602] Bhavna and Saurabh Bhatia. Convergence analysis of optimal iterative family for multiple roots and its applications. *Journal of Mathematical Chemistry*, 62(8):2007–2038, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01640-6`.

Roul:2024:FOC

[3603] Pradip Roul and Vikas Rohil. A fourth-order compact ADI scheme for solving a two-dimensional time-fractional reaction–subdiffusion equation. *Journal of Mathematical Chemistry*, 62(8):2039–2055, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01638-0`.

Belkic:2024:SSS

[3604] Dzevad Belkić and Karen Belkić. Steady spectra of supreme resolution and lowest noise in high-order optimized derivative fast Fourier transform for ovarian NMR spectroscopy. *Journal of Mathematical Chemistry*, 62(8):2056–2080, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01643-3`.

Martinez-Araya:2024:CDDb

[3605] Jorge I. Martínez-Araya. Correction: The dual descriptor potential. *Journal of Mathematical Chemistry*, 62(8):2081–2082, September 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01661-1`. See [3562, 3563].

Fernandez:2024:RRV

[3606] Francisco M. Fernández. On the Raleigh–Ritz variational method. nonorthogonal basis set. *Journal of Mathematical Chemistry*, 62(9):2083–2089, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01644-2`.

Kaur:2024:CSC

[3607] Manpreet Kaur and Mamta Kapoor. A comparative study of cubic UAT and cubic UAH tension B-splines DQM for convection–diffusion equation: a statistical validation. *Journal of Mathematical Chemistry*, 62(9): 2090–2128, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01641-5`.

Medvedeva:2024:VES

[3608] Marina A. Medvedeva and T. E. Simos. A very efficient and sophisticated fourteenth-order phase-fitting method for addressing chemical issues. *Journal of Mathematical Chemistry*, 62(9):2129–2159, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01636-2`.

Diaz-Marin:2024:IME

[3609] Homero G. Díaz-Marín and José L. Sánchez-Ponce. Intraspecific and monotone enzyme catalysis with oscillatory substrate and inhibitor supplies. *Journal of Mathematical Chemistry*, 62(9):2160–2190, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01630-8`.

Hu:2024:CRI

[3610] Xianfa Hu, Wansheng Wang, Bin Wang, and Yonglei Fang. Cost-reduction implicit exponential Runge–Kutta methods for highly oscillatory systems. *Journal of Mathematical Chemistry*, 62(9):2191–2221, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01646-0`.

Sylvia:2024:SCR

[3611] Jasinth Sylvia and Surath Ghosh. Solution of chemical reaction model using Haar wavelet method with Caputo derivative. *Journal of Mathematical Chemistry*, 62(9):2222–2252, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01654-0`.

Srivastava:2024:TPT

[3612] Abhay P. Srivastava, Brijesh K. Pandey, A. K. Gupta, and Anjani K. Pandey. Theoretical prediction of thermoelastic properties of bismuth ferrite by a new approach. *Journal of Mathematical Chemistry*, 62(9):

2253–2264, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01647-z.

Tripathi:2024:TPG

[3613] Shipra Tripathi, Abhi Sarika Bharti, Anjani Kumar Pandey, and Chandra Kumar Dixit. Theoretical prediction of Gruneisen parameter for chalcopyrites. *Journal of Mathematical Chemistry*, 62(9):2265–2279, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01645-1.

Fujisawa:2024:RHF

[3614] Jun Fujisawa. Resonant hexagons in fullerene graphs. *Journal of Mathematical Chemistry*, 62(9):2280–2288, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01650-4.

Tikhonov:2024:MIS

[3615] Nikolay A. Tikhonov. Modeling of isothermal supersaturation of solutions in a porous medium: estimation of it's possible degree. *Journal of Mathematical Chemistry*, 62(9):2289–2303, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01648-y.

Kumari:2024:NHV

[3616] Sarika Kumari, Lok Nath Kannaujiya, Narendra Kumar, Amit K. Verma, and Ravi P. Agarwal. A novel hybrid variation iteration method and eigenvalues of fractional order singular eigenvalue problems. *Journal of Mathematical Chemistry*, 62(9):2304–2325, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01651-3.

Perfileev:2024:TRA

[3617] Michael Perfileev and Vladislav Lyakishev. Theorem on rates of alignment of electronegativities of atoms in the process of formation of a chemical bond in a binary molecule. *Journal of Mathematical Chemistry*, 62(9):2326–2333, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01655-z.

Kirov:2024:EHI

[3618] Mikhail V. Kirov. Entropy of hexagonal ice monolayer and of other three-coordinated systems. *Journal of Mathematical Chemistry*, 62(9):

2334–2345, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01656-y`.

Sivashankar:2024:SCR

[3619] M. Sivashankar, S. Sabarinathan, Hasib Khan, Jehad Alzabut, and J. F. Gómez-Aguilar. Stability and computational results for chemical kinetics reactions in enzyme. *Journal of Mathematical Chemistry*, 62(9): 2346–2367, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01660-2`.

Martinez-Araya:2024:CWL

[3620] Jorge I. Martínez-Araya. Correction: Why local softness and local hypersoftness are more appropriate local reactivity descriptors than dual descriptor and Fukui functions? *Journal of Mathematical Chemistry*, 62(9): 2368–2369, October 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01662-0`. See [3534].

Basak:2024:GES

[3621] Subhash C. Basak and Tanmoy Chakraborty. Guest editorial for the special collection of mathematical chemistry papers. *Journal of Mathematical Chemistry*, 62(10):2371–2372, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01676-8`.

Toropova:2024:PRT

[3622] Alla P. Toropova, Andrey A. Toropov, Ivan Raska, Maria Raskova, and Ramon Carbó-Dorca. The prediction of the retention time of pesticide based on the Monte Carlo method with the use of the vector of the ideality of correlation and correlation weights of local symmetry fragments. *Journal of Mathematical Chemistry*, 62(10):2373–2387, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01517-0`.

Natarajan:2024:CDS

[3623] Ramanathan Natarajan, Claudiu N. Lungu, and Subhash C. Basak. Chirality descriptors for structure-activity relationship modeling of bioactive molecules. *Journal of Mathematical Chemistry*, 62(10):2388–2406, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-

8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01531-2.

Ali:2024:TIT

[3624] Haidar Ali, Didar Abdulkhaleq Ali, Fareeha Liaqat, Muhammad Huzaifa Yaseen, Muhammad Ijaz Khan, Shahid Ali, Norah Almalki, and Barno Sayfutdinovna Abdullaeva. On topological indices of third type of hex-derived networks. *Journal of Mathematical Chemistry*, 62(10):2407–2429, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01555-8.

Saxena:2024:PSC

[3625] Anil Kumar Saxena, Ankit Kumar Gupta, and Karanpreet Singh Bhatia. Physicochemical significance of ChemDraw and Dragon computed parameters: correlation studies in the sets with aliphatic and aromatic substituents. *Journal of Mathematical Chemistry*, 62(10):2430–2455, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01558-5.

Hasani:2024:CTI

[3626] Mehri Hasani and Masoud Ghods. Calculation of topological indices along with MATLAB coding in QSPR analysis of calcium channel-blocking cardiac drugs. *Journal of Mathematical Chemistry*, 62(10):2456–2477, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01570-9.

Gupta:2024:NAK

[3627] Swagata Gupta, Nilanjana Jain, Laxmi Sule, and Nitin S. Sapre. A novel application of Kier–Hall electrotopological descriptors in datamining new HIV-1 non-nucleoside reverse transcriptase inhibitors (NNRTIs) on the basis of chemical similarity. *Journal of Mathematical Chemistry*, 62(10):2478–2501, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01503-6.

Yiarayong:2024:MAD

[3628] Pairote Yiarayong. Multiple-attribute decision making for green sustainable recycling partner selection based on linguistic r, s, t-spherical fuzzy aggregation information. *Journal of Mathematical Chemistry*, 62(10):2502–2539, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01504-5.

Sule:2024:CMS

[3629] Laxmi Sule, Swagata Gupta, Nilanjana Jain, and Nitin S. Sapre. Computational modelling studies on in silico missenses in COVID-19 proteins and their effects on ligand-protein interactions. *Journal of Mathematical Chemistry*, 62(10):2540–2561, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01512-5.

Zhou:2024:AGT

[3630] Ziyun Zhou and Guang Hu. Applications of graph theory in studying protein structure, dynamics, and interactions. *Journal of Mathematical Chemistry*, 62(10):2562–2580, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01511-6.

Das:2024:TIM

[3631] Shibsankar Das, Shikha Rai, and Virendra Kumar. On topological indices of molnupiravir and its QSPR modelling with some other antiviral drugs to treat COVID-19 patients. *Journal of Mathematical Chemistry*, 62(10):2581–2624, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01518-z.

Chen:2024:TPS

[3632] Hanlin Chen. Tutte polynomials for some chemical polycyclic graphs. *Journal of Mathematical Chemistry*, 62(10):2625–2650, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01516-1.

Manohara:2024:FWC

[3633] G. Manohara and S. Kumbinarasaiah. Fibonacci wavelet collocation method for the numerical approximation of fractional order Brusselator chemical model. *Journal of Mathematical Chemistry*, 62(10):2651–2681, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01521-4.

Carbo-Dorca:2024:QMS

[3634] Ramon Carbó-Dorca. QSPR in molecular spaces: ordering data, de- & re-constructing molecular similarity matrices, building their isomet-

ric vectors defining statistical-like momenta of molecular polyhedra, and analyzing the structure of a quantum QSPR operator. *Journal of Mathematical Chemistry*, 62(10):2682–2708, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01501-8`.

Xu:2024:MEC

[3635] Changjin Xu, Yingyan Zhao, Jinting Lin, Yicheng Pang, Zixin Liu, Jianwei Shen, Youxiang Qin, Muhammad Farman, and Shabir Ahmad. Mathematical exploration on control of bifurcation for a plankton-oxygen dynamical model owning delay. *Journal of Mathematical Chemistry*, 62(10): 2709–2739, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01543-y`.

Das:2024:EGA

[3636] Kinkar Chandra Das and Sourav Mondal. On exponential geometric–arithmetic index of graphs. *Journal of Mathematical Chemistry*, 62(10): 2740–2760, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01542-z`.

Akdemir:2024:ABC

[3637] S. Akdemir, S. Özay, and E. Öztekin. Asymptotic behavior of Clebsch–Gordan coefficients. *Journal of Mathematical Chemistry*, 62(10):2761–2775, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01544-x`.

Sule:2024:SIM

[3638] Laxmi Sule, Swagata Gupta, Nilanjana Jain, and Nitin S. Sapre. In silico induction of missense mutation in NNRTI protein: computational modelling and stability study of modelled proteins. *Journal of Mathematical Chemistry*, 62(10):2776–2797, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-023-01545-w`.

Ahmad:2024:OST

[3639] Jamshad Ahmad, Zulaikha Mustafa, and Muhammad Nadeem. Optical solutions to the truncated M-fractional Schrödinger–KdV equation via an analytical method. *Journal of Mathematical Chemistry*, 62(10):2798–2815, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01554-9.

Li:2024:SIM

[3640] Shuguang Li, Faisal Sultan, Muhammad Yaseen, Muhammad Shahzad, and El-Sayed M. Sherif. Slow invariant manifold assessment for efficient production of H_2SO_4 by SO_2: a computational approach. *Journal of Mathematical Chemistry*, 62(10):2816–2826, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01565-6.

Das:2024:SOB

[3641] Shayeri Das, Prabhat Ranjan, and Tanmoy Chakraborty. Study of oxide-based nano cluster X_3O_4 (X = Ti, Fe and Zn) for biomedical applications: a CDFT approach. *Journal of Mathematical Chemistry*, 62(10):2827–2843, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01569-2.

Winkler:2024:CRD

[3642] David A. Winkler. Computational repurposing of drugs for viral diseases and current and future pandemics. *Journal of Mathematical Chemistry*, 62(10):2844–2879, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-023-01568-3.

Kenouche:2024:LRF

[3643] Samir Kenouche and Jorge I. Martínez-Araya. The linear response function $\chi(r, r')$: another perspective. *Journal of Mathematical Chemistry*, 62(10):2880–2888, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01578-9.

Raja:2024:BAA

[3644] Nadar Jenita Mary Masilamani Raja and A. Anuradha. Bonding alkane attributes with topological indices: a statistical intervention. *Journal of Mathematical Chemistry*, 62(10):2889–2911, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01584-x.

Jiang:2024:FOE

[3645] Bo Jiang, Changna Lu, and Yonglei Fang. Fourth-order energy-preserving time integrator for solving the sine-Gordon equation. *Journal*

of Mathematical Chemistry, 62(10):2912–2923, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01586-9`.

Bhattacharjee:2024:RRT

[3646] Apurba K Bhattacharjee. A review on recent theoretical approaches made in the discovery of potential Covid-19 therapeutics. *Journal of Mathematical Chemistry*, 62(10):2924–2942, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01626-4`.

Adel:2024:CSS

[3647] Moein Adel, Peyman Keyhanvar, Masoumeh Zahmatkeshan, Zahed Tavangari, and Neda Keyhanvar. A comparative simulation study of piezoelectric properties in zigzag and armchair boron nitride nanotubes: by discovering a pioneering protocol. *Journal of Mathematical Chemistry*, 62(10):2943–2958, November 2024. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01635-3`.

Bason:2025:NHP

[3648] Gregory L. Bason and B. Cameron Reed. Normalizing the hydrogenic polar solutions $\Theta_{\ell m}(\theta)$ without associated Legendre polynomials. *Journal of Mathematical Chemistry*, 63(1):1–13, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01649-x`.

Tiongson:2025:PEP

[3649] Jaysie Mher G. Tiongson, Dylan Antonio S. J. Talabis, and Lauro L. Fontanil. Positive equilibria of power law kinetic systems with kinetics-based decompositions. *Journal of Mathematical Chemistry*, 63(1):14–38, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01657-x`.

Kapoor:2025:NSO

[3650] Mamta Kapoor. Numerical solution of one- and two-dimensional Hyperbolic Telegraph equation via Cubic–Quartic Hyperbolic B-Spline DQM: a statistical validity. *Journal of Mathematical Chemistry*, 63(1):39–72, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01652-2`.

Flores-Gomez:2025:QRD

[3651] L. Flores-Gómez and N. Flores-Gallegos. Q-rényi's divergence as a possible chemical similarity criterion. *Journal of Mathematical Chemistry*, 63(1):73–95, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01663-z`.

Furtula:2025:PFI

[3652] Boris Furtula and Mert Sinan Oz. On properties of the first inverse Nirmala index. *Journal of Mathematical Chemistry*, 63(1):96–104, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01665-x`.

Kumari:2025:NSL

[3653] Shweta Kumari and Mani Mehra. Numerical solution to loaded difference scheme for time-fractional diffusion equation with temporal loads. *Journal of Mathematical Chemistry*, 63(1):105–131, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01658-w`.

Mishra:2025:AUM

[3654] Saurav Mishra, Brijesh Kumar Pandey, and Jyoti Gupta. Advancing understanding of molecular interactions: computational studies on DNA nucleobases and gold nanoparticles using density functional theory. *Journal of Mathematical Chemistry*, 63(1):132–149, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01659-9`.

Gaur:2025:FPI

[3655] Priyanshi Gaur, Brijesh Kumar Pandey, and Priyanshu Srivastava. First-principle insight on the electronics and structural properties of lanthanide metal doped $BaZrO_3$. *Journal of Mathematical Chemistry*, 63 (1):150–160, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01666-w`.

Yang:2025:DBS

[3656] Ying Yang and Jing Guo. Dynamical behaviors of a stochastic multi-molecule biochemical reaction model with Ornstein–Uhlenbeck process. *Journal of Mathematical Chemistry*, 63(1):161–180, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL https://link.springer.com/article/10.1007/s10910-024-01653-1.

Yukalov:2025:RPM

[3657] V. I. Yukalov and S. Gluzman. Resolving the problem of multiple control parameters in optimized Borel-type summation. *Journal of Mathematical Chemistry*, 63(1):181–209, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01669-7.

Boix:2025:SRN

[3658] Macarena Boix, Begoña Cantó, and Maria T. Gassó. Stability of a reactor with niederlinski criterion using RGA matrices. *Journal of Mathematical Chemistry*, 63(1):210–221, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01672-y.

Tripathi:2025:TQS

[3659] Shipra Tripathi, Abhi Sarika Bharti, Kailash Narayan Uttam, C. K. Dixit, and Anjani K. Pandey. Thermodynamical quantities of silver mono halides from spectroscopic data. *Journal of Mathematical Chemistry*, 63(1):222–236, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01664-y.

Chawla:2025:NAF

[3660] Reetika Chawla, Devendra Kumar, and J. Vigo-Aguiar. Numerical analysis of fourth-order multi-term fractional reaction-diffusion equation arises in chemical reactions. *Journal of Mathematical Chemistry*, 63(1):237–266, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01670-0.

Hellwig:2025:UCD

[3661] Jan Hellwig and Klaus Neymeyr. On the uniqueness of continuous and discrete hard models of NMR-spectra. *Journal of Mathematical Chemistry*, 63(1):267–296, January 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01673-x.

Hong:2025:FRF

[3662] Mei Hong, Chia-Liang Lin, and T. E. Simos. A first-rate fourteenth-order phase-fitting approach to solving chemical problems. *Journal of Mathematical Chemistry*, 63(1):297–331, January 2025. CODEN JMCHEG.

ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01668-8.

Selvi:2025:MMH

[3663] K. V. Tamil Selvi, Navnit Jha, A. Eswari, and L. Rajendran. Mathematical modeling of hydrogen evolution by H^+ and H_2O reduction at a rotating disk electrode: theoretical and numerical aspects. *Journal of Mathematical Chemistry*, 63(2):333–352, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01675-9.

Caffarel:2025:PIQ

[3664] Michel Caffarel. Path integral for the quartic oscillator: an accurate analytic formula for the partition function. *Journal of Mathematical Chemistry*, 63(2):353–382, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01671-z.

Sharma:2025:SAD

[3665] Himani Sharma and Munish Kansal. Stability analysis and dynamical behavior of optimal mean-based iterative methods. *Journal of Mathematical Chemistry*, 63(2):383–405, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01674-w.

Granados:2025:BGM

[3666] Ana Granados, Ana Portilla, Yamilet Quintana, and Eva Tourís. Bounds for the Gutman–Milovanović index and some applications. *Journal of Mathematical Chemistry*, 63(2):406–418, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01677-7.

Saez-Martinez:2025:AGR

[3667] Sol Sáez-Martínez. Analysis of a general reaction-diffusion model using Lie symmetries and conservation laws. *Journal of Mathematical Chemistry*, 63(2):419–434, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01679-5.

IlhadaSilva:2025:MFM

[3668] Marline Ilha da Silva, Joice Chaves Marques, and Adriano De Cezaro. On a multi-fractional model for biogas production for a cellulose-based

substrate. *Journal of Mathematical Chemistry*, 63(2):435–455, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01678-6`.

Preetham:2025:SAA

[3669] M. P. Preetham and S. Kumbinarasaiah. Significance of Arrhenius activation energy on three-dimensional unsteady nanofluid flow with nonlinear thermal radiation and Joule heating via wavelet technique. *Journal of Mathematical Chemistry*, 63(2):456–473, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01680-y`.

Yokus:2025:NDA

[3670] Asif Yokus. Nonlinear dispersion analysis using dynamic traveling wave model in chemical kinetics. *Journal of Mathematical Chemistry*, 63(2):474–491, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01683-9`.

Zhao:2025:ITP

[3671] Li-Cai Zhao. Investigation of thermodynamic properties of bilayer graphene under dual gating with perpendicular magnetic field. *Journal of Mathematical Chemistry*, 63(2):492–501, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01684-8`.

Roul:2025:ECT

[3672] Pradip Roul and Ravi P. Agarwal. An efficient computational technique and its convergence analysis for a class of doubly singular boundary value problems. *Journal of Mathematical Chemistry*, 63(2):502–525, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01685-7`.

Bu:2025:SIP

[3673] Sunyoung Bu and Yonghyeon Jeon. A semi-implicit predictor-corrector methods for time-fractional Benjamin–Bona–Mahony–Burgers equations. *Journal of Mathematical Chemistry*, 63(2):526–545, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01688-4`.

Fang:2025:NEF

[3674] Yonglei Fang, Hengmin Lv, and Xiong You. Novel exponentially fitted two-derivative Runge–Kutta methods for solving the radial Schrödinger equation. *Journal of Mathematical Chemistry*, 63(2):546–577, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01681-x`.

Phantu:2025:CCM

[3675] Suganya Phantu and Panawan Suttiarporn. CMMSE: a comparison of model fitting using different response surface designs for optimizing microwave-assisted simultaneous distillation and extraction in Khlu herbal tea essential oil production. *Journal of Mathematical Chemistry*, 63(2):578–595, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01691-9`.

Dwivedi:2025:FHO

[3676] Himanshu Kumar Dwivedi and Rajeev. Fast high-order linearized exponential methods for efficient simulation of 2D time-fractional Burgers equation in polymer solution dynamics. *Journal of Mathematical Chemistry*, 63(2):596–625, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01682-w`.

Taneja:2025:RHO

[3677] Komal Taneja, Komal Deswal, Devendra Kumar, and J. Vigo-Aguiar. A robust and higher order numerical technique for a time-fractional equation with nonlocal condition. *Journal of Mathematical Chemistry*, 63(2):626–649, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01690-w`.

Guseinov:2025:CEI

[3678] I. I. Guseinov and B. A. Mamedov. Correction to: Evaluation of incomplete gamma functions using downward recursion and analytical relations. *Journal of Mathematical Chemistry*, 63(2):650, February 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01686-6`. See [938].

Liu:2025:NSO

[3679] Lei Liu and Yufeng Xu. Numerical solutions of one-dimensional Gelfand equation with fractional Laplacian. *Journal of Mathematical Chemistry*, 63(3):651–665, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01689-3`.

Cai:2025:EES

[3680] May Cai, Matthias Himmelmann, and Birte Ostermann. Empirically exploring the space of monostationarity in dual phosphorylation. *Journal of Mathematical Chemistry*, 63(3):666–692, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01687-5`.

Kumari:2025:UCT

[3681] Parvin Kumari, Devendra Kumar, and Dumitru Baleanu. An ϱ - uniformly convergent technique for singularly perturbed problems, with an interior turning point occurring in chemical processes. *Journal of Mathematical Chemistry*, 63(3):693–714, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01692-8`.

Lv:2025:IEM

[3682] Junlan Lv, Jianfei Huang, and Sadia Arshad. An improved Euler method for time fractional nonlinear subdiffusion equations with initial singularity. *Journal of Mathematical Chemistry*, 63(3):715–730, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01693-7`.

Abreu-Blaya:2025:IIS

[3683] Ricardo Abreu-Blaya, Jorge Batanero, José M. Rodríguez, and José M. Sigarreta. On irregularity integral Sombor indices: theory and chemical applications. *Journal of Mathematical Chemistry*, 63(3):731–748, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01697-3`.

Quapp:2025:MDT

[3684] Wolfgang Quapp and Josep Maria Bofill. Mechanochemistry of degree two. *Journal of Mathematical Chemistry*, 63(3):749–762, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL https://link.springer.com/article/10.1007/s10910-024-01696-4.

Belkic:2025:IED

[3685] Dzevad Belkić. Interference effects in differential cross sections for two-electron transfer. *Journal of Mathematical Chemistry*, 63(3):763–786, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01699-1.

Arockiaraj:2025:MTG

[3686] Micheal Arockiaraj, J. Celin Fiona, C. I. Arokiya Doss, and Krishnan Balasubramanian. Mathematical techniques for graph descriptors, entropies, spectra, and properties of oxalate-based metal organic frameworks. *Journal of Mathematical Chemistry*, 63(3):787–815, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01695-5.

Chang:2025:REU

[3687] Shih-Hsiang Chang. Regions of existence and uniqueness for singular nonlinear diffusion problems. *Journal of Mathematical Chemistry*, 63 (3):816–828, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01700-x.

Zhao:2025:MDS

[3688] Haichao Zhao and Haoran Wang. Molecular dynamics simulation of the mechanical properties of multi-walled nanotube comprising x-graphene and y-graphene with different stacking orders. *Journal of Mathematical Chemistry*, 63(3):829–851, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01698-2.

Tan:2025:ICP

[3689] Dan Tan, Haiming Liu, Chia-Liang Lin, and T. E. Simos. Improving chemical problem-solving through the use of a fourteenth-order phase-fitting method. *Journal of Mathematical Chemistry*, 63(3):852–887, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01694-6.

You:2025:PFR

[3690] Jing You and Gaihui Guo. Pattern formation for a reversible biochemical reaction model with cross-diffusion and michalis saturation. *Journal of Mathematical Chemistry*, 63(3):888–910, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01705-0`.

Fernandez:2025:RRM

[3691] Francisco M. Fernández. On the Rayleigh–Ritz method. *Journal of Mathematical Chemistry*, 63(3):911–918, March 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01706-z`.

Lin:2025:AFO

[3692] Chia-Liang Lin and T. E. Simos. The application of a fourteenth-order phase-fitting approach to enhance chemical problem-solving. *Journal of Mathematical Chemistry*, 63(4):919–961, April 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-024-01701-w`.

Singh:2025:IRW

[3693] Randhir Singh, Prabal Datta, Vandana Guleria, and Nirupam Sahoo. Investigation of real-world second-order singular differential equations by optimal homotopy analysis technique. *Journal of Mathematical Chemistry*, 63(4):962–981, April 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01703-2`.

Balasubramanian:2025:VFC

[3694] Krishnan Balasubramanian. Vertex and face colorings of dodecahedron and its distortions for all irreducible representations: insights into dynamic chirality, pentagonal, Jahn–Teller and elongated distortions. *Journal of Mathematical Chemistry*, 63(4):982–1034, April 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01704-1`.

Singh:2025:NTS

[3695] Satpal Singh, Devendra Kumar, and J. Vigo-Aguiar. Numerical treatment of singularly perturbed turning point problems with delay in time. *Journal of Mathematical Chemistry*, 63(4):1035–1064, April 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01707-y`.

Eshaghi:2025:OAP

[3696] AliReza Eshaghi and Zeinab Pouransari. Optimizing Arrhenius parameters for multi-step reactions via metaheuristic algorithms. *Journal of Mathematical Chemistry*, 63(4):1065–1092, April 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01710-3`.

Belkic:2025:ODF

[3697] Dzevad Belkić and Karen Belkić. Optimized derivative fast Fourier transform: Splitting singlet-appearing resonances to genuine multiplets in ovarian NMR spectra from encoded time signals. *Journal of Mathematical Chemistry*, 63(4):1093–1115, April 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01709-w`.

Dubinov:2025:EST

[3698] Alexander E. Dubinov. Einstein–Smoluchowski-type relations for real gases. *Journal of Mathematical Chemistry*, 63(4):1116–1125, April 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01711-2`.

Hristov:2025:ASD

[3699] Jordan Hristov. Approximate solutions to a degenerate reaction–diffusion model: a pragmatic sharp front approach. *Journal of Mathematical Chemistry*, 63(4):1126–1153, April 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01713-0`.

Balasubramanian:2025:CRW

[3700] Krishnan Balasubramanian. Combinatorics of random walks on graphs and walk-entropies: generalized Petersen and isomerization graphs. *Journal of Mathematical Chemistry*, 63(5):1155–1188, May 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01712-1`.

Fan:2025:FBF

[3701] Xin Fan and Ji-Teng Jia. Fast breakdown-free algorithm for computing the determinants of a generalized comrade matrix. *Journal of Mathematical Chemistry*, 63(5):1189–1210, May 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01714-z`.

Li:2025:FAR

[3702] Su-Mei Li, Xin Fan, and Yi-Fan Wang. Fast and accurate recursive algorithms for solving cyclic tridiagonal linear systems. *Journal of Mathematical Chemistry*, 63(5):1211–1228, May 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01716-x`.

Surendran:2025:TSM

[3703] Akash Surendran, Krisztina Zsigmond, Kenneth López-Pérez, and Ramón Alain Miranda-Quintana. Is the Tanimoto similarity a metric? *Journal of Mathematical Chemistry*, 63(5):1229–1240, May 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01721-0`.

Sylvia:2025:NSC

[3704] Jasinth Sylvia and Surath Ghosh. Numerical study of a chemical clock reaction framework utilizing the Haar wavelet approach. *Journal of Mathematical Chemistry*, 63(5):1241–1286, May 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01719-8`.

Taneja:2025:NSF

[3705] Komal Taneja, Reetika Chawla, Devendra Kumar, and J. Vigo-Aguiar. Numerical study of the fractional fourth-order evolution problems with weak singularity arises in chemical systems. *Journal of Mathematical Chemistry*, 63(5):1287–1311, May 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01718-9`.

Holba:2025:CLE

[3706] Pavel Holba. Conservation laws for extended generalized Cahn–Hilliard–Kuramoto–Sivashinsky equation in any dimension. *Journal of Mathematical Chemistry*, 63(5):1312–1322, May 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01717-w`.

Szabo:2025:ASR

[3707] Rebeka Szabó and Gábor Lente. Analytical solutions for the rate equations of some two-step kinetic schemes including a reversible first order later step. *Journal of Mathematical Chemistry*, 63(5):1323–1341, May 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897

(electronic). URL https://link.springer.com/article/10.1007/s10910-025-01726-9.

Fernandez:2025:ARR

[3708] Francisco M. Fernández. On the application of the Rayleigh–Ritz method to a projected Hamiltonian. *Journal of Mathematical Chemistry*, 63(6): 1343–1351, July 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01725-w.

Balasubramanian:2025:CFM

[3709] Krishnan Balasubramanian. Combinatorial S-function method for relativistic spinor states of $5g$-row dimers: (e-121)$_2$ to (e-137)$_2$. *Journal of Mathematical Chemistry*, 63(6):1352–1394, July 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01715-y.

Balasubramanian:2025:CCD

[3710] Krishnan Balasubramanian. Combinatorics of colorings of Dürer graph, Dürer solid in *Melencolia I*, their heptagonal analogues and antiprisms for all irreducible representations: chirality, dynamics, NMR spectra and enumerations. *Journal of Mathematical Chemistry*, 63(6):1395–1446, July 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01720-1.

Faria:2025:SOL

[3711] Henrique Antonio Mendonça Faria, Jorge Manuel Vieira Capela, and Fabio Roberto Chavarette. Simulation of optimal linear control for stabilizing chaotic behavior in a chemical reaction model. *Journal of Mathematical Chemistry*, 63(6):1447–1460, July 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01723-y.

Huang:2025:SPE

[3712] Jian Huang, Zhongdi Cen, and Aimin Xu. A simplified a posteriori error analysis of a second-order difference scheme for a singularly perturbed convection–diffusion problem. *Journal of Mathematical Chemistry*, 63 (6):1461–1474, July 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01729-6.

Bhuvaneswari:2025:EAA

[3713] M. Bhuvaneswari, V. Vinoba, and G. Hariharan. An efficient approximation algorithm for the nonlinear reaction: diffusion equations in an electro catalytic thin film models using Hosoya polynomials. *Journal of Mathematical Chemistry*, 63(6):1475–1495, July 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01728-7`.

Lin:2025:LOE

[3714] Chia-Liang Lin and Theodore E. Simos. Low-order efficient Adams–Bashforth–Moulton methods for first-order IVPs with oscillating solutions. *Journal of Mathematical Chemistry*, 63(6):1496–1522, July 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01727-8`.

Viswanathan:2025:CFR

[3715] Balakrishnan Viswanathan and Darien DeWolf. Closed-form representations of the Coulomb integral over hydrogenic orbitals. *Journal of Mathematical Chemistry*, 63(6):1523–1550, July 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01734-9`.

Tiebekabe:2025:CLF

[3716] Pagdame Tiebekabe and Ismaïla Diouf. Correction to: Linear forms in logarithms and the mathematical method of diophantine equations: applications in chemistry and physics. *Journal of Mathematical Chemistry*, 63(6):1551–1553, July 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01722-z`. See [3283].

Tandon:2025:FSG

[3717] Hiteshi Tandon and Tanmoy Chakraborty. Floating spherical Gaussian orbital model: a brief overview. *Journal of Mathematical Chemistry*, 63(7):??, August 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01735-8`.

Quapp:2025:MMS

[3718] Wolfgang Quapp, Josep Maria Bofill, and Sinan Keten. To a mechanical model of synthetic catch-bonds. *Journal of Mathematical Chemistry*, 63(7):1555–1565, August 2025. CODEN JMCHEG. ISSN 0259-

9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01731-y.

Pino-Rios:2025:CBD

[3719] Ricardo Pino-Rios. Condensed-to-bond dual descriptor for the analysis of electron density rearrangement in π-conjugated compounds. *Journal of Mathematical Chemistry*, 63(7):1566–1587, August 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01730-z.

Belkic:2025:BSR

[3720] Dzevad Belkić and Karen Belkić. Beyond the SNR-resolution uncertainty principle: Optimized derivative fast Fourier transform for NMR diagnostics in medicine. *Journal of Mathematical Chemistry*, 63(7):1588–1597, August 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01733-w.

Bai:2025:MTP

[3721] Xilong Bai, Zhensheng Lu, and Liu Long. Magnetic and thermal properties of phosphorene quantum rings. *Journal of Mathematical Chemistry*, 63(7):1598–1635, August 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01732-x.

Arnrich:2025:NSA

[3722] Steffen Arnrich and Grit Kalies. The numerical solution of the adsorption integral equation with Langmuir-kernel. Part 1: approximations. *Journal of Mathematical Chemistry*, 63(7):1636–1649, August 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01724-x.

Morales-Bayuelo:2025:LSL

[3723] Alejandro Morales-Bayuelo. Local softness and local molecular quantum similarity relationship: quantification of the local softness within a molecular ensemble. *Journal of Mathematical Chemistry*, 63(8):??, September 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-024-01702-9.

Xu:2025:CO

[3724] Rong Xu, Bin Sun, and T. E. Simos. Comments on "The use of a multistep, cost-efficient fourteenth-order phase-fitting method to chemistry

problems" and "An effective multistep fourteenth-order phase-fitting approach to solving chemistry problems". *Journal of Mathematical Chemistry*, 63(8):1679–1685, September 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01708-x`.

Kumari:2025:ANS

[3725] Parvin Kumari, Jesus Vigo-Aguiar, and Garima Agarwal. Analysis and numerical solution of singularly perturbed partial differential equations with large spatial delays and integral boundary conditions: applications in chemical and catalytic systems. *Journal of Mathematical Chemistry*, 63(8):1686–1688, September 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01737-6`.

Kumar:2025:PEC

[3726] Jitender Kumar, Vikas Kumar, and Norqulova Ziyoda Nabi Qizi. Pattern evolution of coupled reaction–diffusion models arises in chemical systems using modified trigonometric cubic B-spline functions. *Journal of Mathematical Chemistry*, 63(8):1689–1714, September 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01736-7`.

Inyang:2025:QEV

[3727] Etido P. Inyang. Quantum expectation values and Shannon entropy in diatomic molecular systems. *Journal of Mathematical Chemistry*, 63(8):1715–1731, September 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01738-5`.

Meral:2025:MMA

[3728] Gülnihal Meral and Derya Altintan. Mathematical modeling and analysis for Michaelis–Menten kinetics. *Journal of Mathematical Chemistry*, 63(8):1732–1752, September 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01739-4`.

Flores-Gallegos:2025:NAR

[3729] N. Flores-Gallegos and L. Flores-Gómez. A new approach of Rényi's information measures. *Journal of Mathematical Chemistry*, 63(9):1767–1791, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01740-x`.

Lente:2025:DIK

[3730] Gábor Lente. Direction independence as a key property to derive a particle speed distribution in real gases. *Journal of Mathematical Chemistry*, 63(9):1792–1805, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01742-9`.

Dimsey:2025:BMN

[3731] Heath W. Dimsey, Lawrence K. Forbes, and Andrew P. Bassom. The BROCODE model: a novel mathematical model for the Briggs–Rauscher reaction. *Journal of Mathematical Chemistry*, 63(9):1806–1825, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01743-8`.

Yang:2025:HOS

[3732] Fan Yang, Zhida Zhou, and Chaolong Jiang. High-order structure-preserving schemes for the regularized logarithmic Schrödinger equation. *Journal of Mathematical Chemistry*, 63(9):1826–1853, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01741-w`.

Perfileev:2025:WSP

[3733] Michael Sergeevich Perfileev and Vladislav Konstantinovich Lyakishev. Wiener sausage and particle collision frequency factor. *Journal of Mathematical Chemistry*, 63(9):1854–1863, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01745-6`.

Balasubramanian:2025:NIA

[3734] Krishnan Balasubramanian. New insights into aromaticity, Kekulé structures, Dewar structures of armchair versus zigzag carbon nanotubes through delta, matching and spectral polynomials. *Journal of Mathematical Chemistry*, 63(9):1864–1906, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL `https://link.springer.com/article/10.1007/s10910-025-01746-5`.

Belkic:2025:RPC

[3735] Dzevad Belkić and Karen Belkić. Recognized and potential cancer biomarkers in ovarian MRS: Padé quantitative derivative shape estimation without fitting. *Journal of Mathematical Chemistry*, 63(9):1907–1948, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print),

1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01744-7.

Balasubramanian:2025:SPG

[3736] Krishnan Balasubramanian. Spectral polynomials, graph descriptors, spectra, and entropies of cage graphs. *Journal of Mathematical Chemistry*, 63(9):1949–1988, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01747-4. See correction [3737].

Balasubramanian:2025:CSP

[3737] Krishnan Balasubramanian. Correction: Spectral polynomials, graph descriptors, spectra, and entropies of cage graphs. *Journal of Mathematical Chemistry*, 63(9):1989–1992, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01751-8. See [3736].

Amore:2025:TDH

[3738] Paolo Amore and Francisco M. Fernández. On the two-dimensional hydrogen atom in a circular box in the presence of an electric field. *Journal of Mathematical Chemistry*, 63(9):1993–2000, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01750-9.

Medvedeva:2025:ELO

[3739] Marina A. Medvedeva and Theodore E. Simos. Efficient low-order Adams–Bashforth–Moulton trigonometrically-fitted methods. *Journal of Mathematical Chemistry*, 63(9):2001–2022, October 2025. CODEN JMCHEG. ISSN 0259-9791 (print), 1572-8897 (electronic). URL https://link.springer.com/article/10.1007/s10910-025-01748-3.

Kerber:1991:ACF

[3740] Adalbert Kerber. *Algebraic combinatorics via finite group actions*. B. I. Wissenschaftsverlag, Mannheim, Germany, 1991. ISBN 3-411-14521-8. 436 pp. LCCN QA171 .K419 1991.

Sternberg:1994:GTP

[3741] Shlomo Sternberg. *Group theory and physics*. Cambridge University Press, Cambridge, UK, 1994. ISBN 0-521-24870-1. xiii + 429 pp. LCCN QC20.7.G76 S86 1994. URL http://www.loc.gov/catdir/description/cam041/94119781.html; http://www.loc.gov/catdir/samples/cam034/94119781.html; http://www.loc.gov/catdir/toc/

cam041/94119781.html; http://www.zentralblattmath.org/zmath/en/search/?an=0816.53002.

Kerber:1999:AFG

[3742] Adalbert Kerber. *Applied finite group actions*, volume 19 of *Algorithms and combinatorics*. Springer-Verlag, Berlin, Germany / Heidelberg, Germany / London, UK / etc., second edition, 1999. ISBN 3-540-65941-2 (hardcover). ISSN 0937-5511. xxv + 454 pp. LCCN QA174.2 .K47 1999. URL http://www.loc.gov/catdir/enhancements/fy0815/99039852-d.html; http://www.loc.gov/catdir/enhancements/fy0815/99039852-t.html.