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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
FAX: +1 801 581 4148
E-mail: beebe@math.utah.edu, beebe@acm.org, beebe@computer.org (Internet)
WWW URL: http://www.math.utah.edu/~beebe/
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Title word cross-reference

\( (N - 1) [ACD^{+13a}, ACD^{+13b}] \quad (\sigma^3, \lambda^3) [TR12] \quad (\sigma^3, \lambda^3) [TR12] \quad + \quad [CXW14, GTK10, NMLD13] \quad 0 [UD12] \quad 1 [MG15, TS15b] \quad 1 - n [CYG^{+15}] \quad 10 [AC11b, TS15b] \quad 13 [WYGW12] \quad 15 [AC11b] \quad 17 [GZZ12] \quad 18 [LW16] \quad 2 \quad [CWT^{+12}, GSS13, MSBF16, MH10, SJD14, WvRSM14, YDL^{+10}] \quad 20 \quad [AC11b, LYL16, YVEI^{+17}] \quad 24 [TS15b] \quad 3 \quad [AARP17, CM16, DVVP14, GMMH^{+16}, GSS13, GPK12, LTT16, MG15, MA16, MYT^{+14}, MSSP17, PSS14, RVCFF13, TS15b, YLL11] \quad 4 \quad [AFSW16, GWJJ12, ZTH^{+15}] \quad 4d [Hil13] \quad 4f [Hua16] \quad 4 \times 1 [LGKS17] \quad 4 \times 4 \quad [SH14] \quad 5 [APY^{+16}, LZH16, YLL11] \quad 5^{12} [MKH15] \quad 6 \quad [MCAY15, Rab12, TSZQ12] \quad 6^2 [MKH15] \quad 6^3 [MKH15] \quad 6^4 [MKH15] \quad 8 \quad [TN12] \quad 8 \times 2 [LGKS17] \quad 2 + 2 [LXFC17] \quad 5 + 1 [YZL^{+15}] \quad 5 + 2 \quad [LXFC17] \quad [n] [uLhY11] \quad + [DDM^{+15}, FD16, LCL^{+10}, LdSRR16, LCWW10, RLA^{+11}, RRF11, SFBT17, UT14, YCGA10, YZ15b, ZCK^{+16}, ZWY^{+10a}].\)
WKC10a, YHK15, ZXS+10, ZLY+16, ZBB16]. 48 [YW12]. 5 [Bac12, CG12, Ibr17, JLS+10, PBE16, RDT14, SJD11, STS+10, SSX+14, XFX+16]. 56 [TFQ+11]. 57 [SNKS10]. 5a [GWT+17]. 6
[BTMS12, BS16b, Cas14, CG12, GBGR16, KV14, LLL+12, OPR16, SWMV10, SSX+14, Tak11, WMW11, WRT+17, YHK15, YOPB16, YHW17]. 60 [KP10, LLC17, MSV16, RLA+11, SKMS13, SBW12, TFQ+10, WLW+10, WCY+11, WL14, YDGZ15]. 62 [GWT+17]. 7 [GBGR16, OPR16]. 70
[ZSL+11]. 71 [VL17b]. 76 [ZYG+14]. 8
[WWKS16, WCL+11, YW12, YOPB16]. 84 [FL15]. 89 [SNKS10]. 9 [Cas14]. 980 [WTH+16]. A [GK15a, SK15a, WGN+16, SK12, SK17, Zha12b, Zha12a].
\text{ax} [SNDK16]. \text{CARBO} [PLH16]. d [Sch13]. \text{glyc} [PFVL14]. k [GM17]. H
[HCD]. 10
[HNN]. N
[HOM+16, LGW12, RWR+13, YZGS14b, Yu12b, Yu12a, ZYR+15, ASS10, AC11b, CKL+11, GTF10, GWJ11, GWJJ12. JM11, JLH+14, MCAY15, NC14, PZBA13, Rab12, RVCFF13, SN16a, TN12, Tak10, Tak11, TSZQ12, TS15b, WYGW12, XhD15, YVEI+17, vSGP10]. + [ABB+12, ABB+13]. −
[GZZ12, GWJJ12]. −/0 [YLL11]. nV [PZBA13]. x [CWT+12, LZT10, SB11].
\text{ze} [YZWC11]. a [TN10].
[CCHO14, DBG11, DB12, FFA14, HPT16a, HHT+13a, HHT+13b, LJW+11b, LDH+14, NDU14, RWR+13, SWMV10, SH14, SKY+11, WXL+12, WCAH10, XLYZ10, YR13, YZL+15, ZYR+15, ZKH+10, LFB14]. B [GWX+12]. 1
[HSH15]. β [AKMT11, BLS10, CYY+17, CCOH14, DBG11, HPT16a, IO13b, LLvG10, LJW+11b, LvG13a, LvG13c, LJL+11, NGAS17, yOaCG10, SKY+11, WS10, WXL+12, XWSW13, YZ17, XZ11, ZBP11, ZP13, ZKH+10].
\beta_2 [CV12, VKC10, LLHM16]. c [TN10].
[BH13, LZX+15b, RAGL11, YHK15, BZHI4]. . . . . .
[CROB16, VVJ15, WvRSM14]. . . . . . [CCCLCGRO14]. . . . . . . . [YZZ+17]. \chi [DPSL16]. \chi_1 [SZBM13]. \chi_2 [SZBM13]. d
[CAT+13, JSW15, KTK17, MCK17a, SM17, TDKT10]. d^6 [TS15a]. d_4 [Kow11]. e^− [HBL12]. e_2 [WCY+11]. \eta^2 [RHPWS13]. \eta^6 [ZCK+16]. f
[CAT+13, JSW15, MCK17a, TDKT10]. f^n [BBG+18]. γ
[BTB+11, DBG11, YLCX10]. J [KNP+12, LHZ+11]. k [Hug14, YS15]. κ
[YRSS10]. λ [BH15]. λ^3 [SLT14]. λ^N [XHLH16]. ↔ [RSK+15]. m = 2
[TS15b]. m = 2, 3 [TS15b]. \mu [RHPWS13]. N
[AARP17, HPT17, JSW10, KYCL11, KYKR15, SKK11, LHL+10, LXZ+10, MB16, PHT17, QZM11, RF15, YLZ+10, ZYW+10a, ZBP11, dSDLBW17, BLBG+13, BS10b, HCB11, JLH+14, LXFC17, RRF11]. n + m = 4 [XhD15].

n + m ≤ 3 [GTT10]. n = 0 [MCAY15]. n = 1
[GWJJ12, Rab12, RVCFF13, TN12, TSZQ12, YLL11, TS15b]. n = 1, 2
[ABB+12, ABB+13]. n = 10 [TS15b]. n = 12 [YVEI+17]. n = 2
[WYGW12, TS15b]. n = 4 [GZZ12, TS15b]. n = 5 [AC11b]. n ≤ 20 [ASS10].

n ≤ 25 [Tak11]. n ≤ 55 [Tak10]. N \log N [AO10]. O(N) [BLS11]. O(N \log N) [FGM11]. p [HNN+17, MCK17b]. π
\[ q = 0, +1, -2 \{X_{\text{Ba}}, R_{\text{CM}^{-1}, 13b}, \rightarrow \}
\]
\[ \{\text{CK}10, \text{Chu}10, \text{GTK}10, \text{H}12, \text{HBL}12, \text{LWD}13, \text{NMLD}13\}, S_1 \{\text{KKL}^{+13}, \sigma \}
\]
\[ \{\text{DPSL}16, \text{GZZM}16, \text{LZL}^{+15b}\}, \sigma \{\text{CZY}11, \text{YWZ}14\}, \text{A}^1 \text{A}’ \{\text{MCLD}10\} \times \{\text{SR}14\}, v = 0 \{\text{LWD}13\}, x = 1 \{\text{CWT}^{+12}, \text{LZTV}10\}.
\]

- \{\text{AKM}11, \text{CAT}^{+13}, \text{DBG}11, \text{JXS}15, \text{LWX}16, \text{LXFC}17, \text{MCK}17a, \text{RHPWS}13, \text{SKY}^{+11}, \text{TDKT}10, \text{YYT}12, \text{ZKH}^{+10}, \text{AMK}11, \text{KYCL}11\}. - 5 \{\text{LL}10c\}, - \text{A} \{\text{Y}JN^{+11}\}, - \text{acceptor} \{\text{MIS}^{+15}\}, - \text{Ac} \{\text{LHL}^{+10}\}, - \text{acetals} \{\text{Y}ZL^{+15}\}, - \text{Aceto-} [\text{SJD}14], - \text{acyethyl} - \text{ZBP}11, - \text{acylation} \{\text{LHL}^{+10}\}, - \text{adrenergic} \{\text{LL}HM16, \text{VK}10\}, - \text{AI} \{\text{YR}13\}, - \text{alkenoyl} \{\text{Y}ZL^{+15}\}, - \text{alumina} \{\text{SH}14\}, - \text{amination} \{\text{Y}Z17\}, - \text{amino} \{\text{ZKH}^{+10}\}, - \text{aminopolycarboxylate} \{\text{CM}D13\}, - \text{arene} \{\text{ZCK}^{+16}\}, - \text{atomic} \{\text{JXS}15\}, - \text{ATPase} [\text{H}10], - \text{azacrown}-5 \{\text{WY}W^{+10a}\}, - \text{barrel} \{\text{yOa}CG10, \text{WXL}^{+12}\}, - \text{based} \{\text{EP}15, \text{PE}16, \text{BPE}16, \text{EBK}13, \text{LFB}14\}, - \text{benzaldehyde} \{\text{Lu}11\}, - \text{bipyridyl} \{\text{KPL}15\}, - \text{block} \{\text{CAT}^{+13}, \text{MCK}17b, \text{TDKT}10\}, - \text{bond} \{\text{CK}1L11\}, - \text{bound} \{\text{XWS}13\}, - \text{butanol} \{\text{BS}10b\}, - \text{butene} \{\text{MSBF}16, \text{WvR}5M14\}, - \text{butyl-} [\text{MG}15], - \text{butylbenzene} \{\text{HCB}11\}, - \text{carboxylates} \{\text{AARP}17\}, - \text{carribose} \{\text{YS}R10\}, - \text{catalyzed} \{\text{Y}XZ1\7\}, - \text{conjugated} \{\text{BLG}^{+13}\}, - \text{coumaric} \{\text{HNN}^{+17}\}, - \text{coulplings} \{\text{LZH}^{+11}\}, - \text{Cu} \{\text{NGA}17\}, - \text{curcumin} \{\text{AMK}11\}, - \text{cyclodextrin} \{\text{DBG}11\}, - \text{dimensional} \{\text{MB}16\}, - \text{dimethylaminophenyl} \{\text{YL}Z^{+10}\}, - \text{effect} \{\text{RWR}^{+13}\}, - \text{electron} \{\text{KTK}17, \text{LW}16, \text{LYL}16, \text{HPT}17, \text{PHT}17\}, - \text{erythrose} \{\text{SM}17\}, - \text{expanded} \{\text{ML}Q^{+12}\}, - \text{F}12a \{\text{MLCD}11\}, - \text{form} \{\text{GW}X^{+12}\}, - \text{glucosamine} \{\text{ZBP}11, \text{ZP}13\}, - \text{glycine} \{\text{DB}12\}, - \text{H} \{\text{LJW}^{+11b}\}, - \text{hairpin} \{\text{LJW}^{+11b}\}, - \text{helices} \{\text{HHT}^{+13a}, \text{HHT}^{+13b}\}, - \text{helix} \{\text{CC}OH14, \text{WX}L^{+12}\}, - \text{heptane} \{\text{R}RF11\}, - \text{heterocyclic} \{\text{KY}K15, \text{LX}Z^{+10}, \text{RF}15, \text{dSD}LBNB17\}, - \text{hole} \{\text{GZZM}16, \text{LZL}^{+15b}\}, - \text{hydrogenase} \{\text{GS}11\}, - \text{hydroxyl-dimethylnitrosamine} \{\text{FFA}14\}, - \text{hydroxybutyrate} \{\text{SJD}14\}, - \text{hydroxymethylfurural} \{\text{APY}^{+16}\}, - \text{hydroxysteroid} \{\text{ZX}11\}, - \text{inhibitor} \{\text{LJJ}^{+11}\}, - \text{iodes} \{\text{SL}T14\}, - \text{ keto} \{\text{LYZ10}\}, - \text{LEUS} \{\text{BH}15\}, - \text{like} \{\text{WGN}^{+16}\}, - \text{maltose} \{\text{SW}M10\}, - \text{metalloid} \{\text{MMS}16\}, - \text{methyl} \{\text{LZL}^{+16}\}, - \text{methyl-Imidazolium} \{\text{MG}15\}, - \text{methylacetamide} \{\text{KSK}11\}, - \text{methylation} \{\text{QZM}11\}, - \text{methylbenzyl} \{\text{NDG}14\}, - \text{methylformamides} \{\text{JSW}10\}, - \text{montmorillonite} \{\text{B}HB^{+17}\}, - \text{N-benzyl-N-} \{\text{NDG}14\}, - \text{naphthol} \{\text{Hug}14, \text{YS}15\}, - \text{nearest} \{\text{Hug}14, \text{YS}15\}, - \text{nitroaniline} \{\text{ZTH}^{+15}\}, - \text{nucleophile} \{\text{ZYR}^{+15}\}, - \text{alanes} \{\text{Y}Z15b\}, - \text{orbitals} \{\text{MCK}17a\}, - \text{organic} \{\text{AH}10\}, - \text{oxo} \{\text{VB}MA13, \text{RHPWS}13\}, - \text{oxoalkyl-substituted} \{\text{AARP}17\}, - \text{Pd} \{\text{dSD}LBNB17\}, - \text{peptide} \{\text{LV}G10, \text{LVG}13a\}, - \text{peptides} \{\text{LV}G13c, \text{ZKH}^{+10}\}, - \text{peroxy} \{\text{RHPWS}13\}, - \text{phenyl-azacrown-5} \{\text{Z}WY^{+10a}\}, - \text{phosphano} \{\text{KY}K15\}, - \text{phosphoranes} \{\text{TR}12\}, - \text{pinane} \{\text{BLS}10\}, - \text{pinene} \{\text{BLS}10\}, - \text{pleated} \{\text{WCA}H10\}, - \text{point} \{\text{BT}B^{+11}\}, - \text{proline}


5 [ZZWX11, cCVG+14, LL10c, Mor15, Pon10, SOvG12]. 5-b [YLZ+10]. 5'-bridged [ZZWX11]. 5-nitroimidetrazolate-based [ZYL+12]. 5-triazine [WDLG12]. 5-triazines [YPC+10]. 5-triene [ABDGN12]. 53A6
[PFVL14, LGL11]. 54A7 [LvG13c]. 56A6 [PLH16].


7 [ADF+10, MBR+15]. 7-azaindole [YYT12]. 7-tetraene [ABDGN12].

8 [AAC+16]. 8-formyl-7-hydroxycoumarin [LZHH11]. 8R [BG13].


= [ASS+17, CXS10, GPK+16, EPH+15, JLH+14, JJAB16, JJJ16, LDJ+10, LLL+11, LZJ+11, Li14a, Li14b, LGW12, LCWW10, LWD13, MCK17a, MCK17b, PGS+15, PMG+16, Rab12, RDT14, SPS+12, SLJ12, TLDG+12, TFO+11, TG12h, UT15, WWKS16, XhD15, YW12, YS13, YHCS11, ZYLL12, ZLLL12].

Ben17, CCLP12, CSGOA17, CRZ+18, DKE+17, GAI13, GBW+14, GWZX12, HRC13, LC17b, LZZ14, MAK+14, ME10, MFR+17, NHH16, yOTn16, dRL11, RB13a, RCR+16, RDDS10, RR14, SH15, SS16b, VAMS14, VDVR14, WXS+12, WJG+13, WX12, XZSL11, YOMT14, dVZ17, dSAdSL13.

Accurately [Bow16, LFB14, MA16, Zha12b]. ACE [WCDM11, LHL+10].

acetaldehyde [AS11, AAMD+11]. acetals [YZL+15]. acetamides [JSW10].

Aceto [SJ14]. acetohydroxyacid [XLYZ10]. acetonitrile [RS14].

acetyl [ZBP11, ZP13]. acetylacetone [SJWE10]. acetylation [FHK+12, IMK+16, LHL+10].

acetylcholine [SRA17]. acetylene [GRCL12, HSY+11, LT13, Tak10].

achieve [PH17, RAR+11]. achieving [NNK+16]. Achim [Spr10].

acid [BLG11, CYY+17, CC18b, CFC15, CM16, CB11d, FD14, FZL+15, Fel10, FP17b, FCE15, GRL+11, GRL+12, HPT16a, HGY15, HCP15, KLS10, KMLS10, LBC+12, LXL+11, LFM12, LP11b, LPMT17, MSLS10, MRO17, NHF+10, OXW16, PHDH13, SISK10, SZBM13, SBW12, SV11, TL16, VMPS17, WC14, WG12, XVN17, ZSB+11, ZWP11, ZHHX11].

acid-catalyzed [CYY+17]. acid-water [TL16].

acid/base [VMPS17]. acidic [APY+16, YDX16]. acidities [ALK+15]. acidity [CRZ+18, CPK12].


Activation [Niz13, AALCM11, DR11, DSM+11, FB12, MRR11, MBFG15, TS15a, WC11, XLYZ10, YXZZ17]. activation-strain [FB12]. activator [BM12].

active [AIGP15, Cas13, DPB+12, LZTV10, PDC+16, SCSW13]. active-space [PDC+16]. actives [EOO+16]. activity [BPC13, DXL+10, GA13, GHL17, GFPSD17, MJLV14a, RCM+13b, SLY+10, TD10, TTB+11, YB13, ZsA10].

acute [TTL+12]. acyclic [ZKH+10]. acyl [PS10]. adamantane [EHSP16].

adamantane-based [EHSP16]. adapted [FF11, SSSM15, TH13, YKH15].

Adaptive [ISK14, KEMP17, LZS+17, AOW11, BGR13, DSK17, FHMB15, HDM+15, MJ14, MBFP15, MJG+15, OZ14, PN13, SNS13, WMW+10].


adrenergic [CV12, LLMH16, VKC10]. adsorbate [GBS+17]. adsorbate-induced [GBS+17]. adsorbed [MCF10, PXXW10, SLLL13, SIG+15]. adsorbents [HVS16]. Adsorption [CCJ+11, FVP14, HB15, KD10, LH14b, PH12, AS15a, BS16b, CMM18, CR14, cCVG+14, Hei10, LL13a, LPK16, LPLS16, LZ14, LT14, LCM+14, NPP13, PGC12, PLZ17, RHHN10, SH14, SDB+16, SKTT11, SYZ+17, VS14].

affinity
[CG15, CZAF17, DLZ15, MCK17a, SSP+13, VL17a, ZJZM13, ZYvIZ14].


algebraic-diagrammatic [YD17]. Algorithm [WM12, AMGB10, AM10, AYYO17, BW11a, BYE+16, BDdS13, CM13a, CDBM11, CVT+11, CM13b, CB11b, DS15, DJ13, DLSA14, DZA11, FRLN10, GFG11, GPE13, GBFD12, HTS15, HEMCZE+14, HQC16, HKR+14, Hug14, Ish10, IHJ+13, JPC11, KK17a, KNN16, KN17, KDT+12, LZX16, LZL+13, LZLMP16, LZS+17, LLLJ12, LTA+11, LMA15, NYN17, NC12, NG10, dRL11, PS17, RMPAM15, Ras17, RSL16, SRSLO15, SYH12, SMMW09, SCSW13, SA11, WMW+10, XHLH16, YVEI+17, ZSS+13, vLBR12].
[BD11, MRB14, BCP+10, HPT17, LZS+17, PHT17, SWA13, WES13].
anapole [ZPP+16]. anatase [HRL11]. and/or [KB10, Pog10].
androstenedione [VCM15]. angle [CP10, GBFD12, XML+15].
angle-dependent [CP10]. angles [BKLA13, EJ13, FZY+12, GREA11, LDH+14, OZ14, YZ16].
anisotropy [CGP12, LPLB16, ZLZ14]. ANN [XWW+11]. annealing [RHJ11, SHMO11, SHL+11, ZC14, LMZ11a]. annihilation [BL12].
aplicable [CL16, WGL+11]. Application [AFBR17, BAMR13, BPE16, GCCM15, HTS15, LDG+15, MBA11, MH10, OL13, PAK15, RVP+11, SMP17a, SRS14, SC17, SDL14, SMM+18, VKTRJ15, WH11, ZsA10, vSGP10, CSaDO17, DGP14, Elk16, GLB16, GFG11, GCW16, IUK+11, KFY+13, KSK11, LLHM16, LP11a, LLL+10, LLLC11, LyG13c, MDTD13, PHC13, RZG+13, RCM+13b, SN16a, SLX+15, SYH12, VV14, VK10, WCDM11, You10, AFP13, BD11, CZNA11, Fer13b, Fer13a, FCQGM12, GA13, HYUS11, KUDG12, MCC11, Pet11, PW12, TSQZ12].
Applications [KGHC15, LCPS13, LCA17, APK14, CGPP11, Fel10, GBFD12, HZY+10, HCD+10, IO13b, KKO+16, uLhY11, LJR+12, MG11, SSSM15, SGM+13, ISP+10]. applied [BLG11, CTP13, GKR13, KKR+13, LTT16, Ray13, RKG11, SZTSM10].
Applying [KB11a, ZSL17, CC11]. approach [ACD+13b, BPE16, BVH17, BGR13, CCLP12, CRZ+18, CHEC13, CSX10, DK11, DGP14, DVP14, DFF+15, DHE+12, FRA14, Fer17, FNSF+11, FCCP17, FD16, FSD+18, GPE+13, GZ14, GH16a, HRC13, HDH12, HNX+17, HHBY10, HZS17, JCX10, KV12, KV13, KSK11, KT10, LLTC12, LHI14a, LG14, MZZ11, MGWR12, ME10, Mor15, NO16, OT12, PRP15, PMC+17, PSdPE+10, PH10b, PBE16, PPU10, PFL+16, PKG10, RB12, RVP+11, SLT14, SEF+16, SH11b, SY16a, Sti15, SLL13, SGH+16, SM17, TAG16, TSR+16, VVLG17, XZ11, YKO+11, ZSL17, ZI10, GFG11, ACD+13a]. approaches [BH13, CME11, DBM+17, ECZWD17, HBI+17, LSH+11].

Baoshan [JW12]. bare [SM17]. barrel [LJR+12, yOaCG10, WXL+12].
bonding-induced [YLZ\textsuperscript{+10}]. bonding/back [PKK\textsuperscript{17}]. bonding/back-bonding [PKK\textsuperscript{17}]. bonds [DBG\textsuperscript{+13}, EDI5, FPRS\textsuperscript{14}, HH15, Jab14, JJ16, LZ\textsuperscript{+11}, LZL\textsuperscript{+15}, LZY\textsuperscript{12b}, LDG\textsuperscript{+15}, OOK\textsuperscript{11}, Rob13, SM16\text{a}, SK13, SJ16, YLL11, YKH15, YJ17, ZLY\textsuperscript{+16}]. BonnMag [BBC\textsuperscript{+18}]. Book [Sch10, Spr10]. boost [KV15\text{a}]. borafflourenes [ZQ14]. borane [BEP\text{M14}, Kop15\text{b}, LC10, SJZ\textsuperscript{+15}]. borane-cyclic [LC10]. borates [GWJ\text{W12}]. border [SK12, SK17]. borides [ZWM\text{W10}]. born [AB16\text{b}, BLZ\textsuperscript{+13}, DSF17, FCE15, KCP\text{MG12}, LL10\text{a}, LCH10, PS13, RS\text{B}13, SZ\text{TS}10, SSBW14, VMPS\text{17}, WWKS\text{11}]. boron [BEP\text{M14}, GAMAC\text{14}, LT\text{14}, Oht16, PGC\text{12}, VS\text{14}]. boron-doped [VS\text{14}]. boron-nitride [LT\text{14}]. boryl [LC10]. BOSS [VKTRJ15]. BOSS-Gaussian [VKTRJ15]. Bosutinib [GMASBF16]. both [AST\textsuperscript{+16}, FNS\text{F11}, LX11, TH13]. bottleneck [SRR\text{16}]. bound [FLM11, GPK\textsuperscript{+16}, LFM12, MAK\textsuperscript{+14}, PMG\textsuperscript{+16}, PZA15, XWS\text{W13}]. boundary [KB14\text{a}, Lun12, MT\text{vG12}, NO16, PL14, PS13, Sie15, VECT12]. bounded [Pol13, SL10]. bowls [WL14]. box [Pla11, WS13]. boxB [XHLH16]. Boys [WO15]. bptz [CWT\textsuperscript{+12}]. bpy [LWXC16]. Br [ASS\textsuperscript{+17}, EPH\text{+15}, LDJ\textsuperscript{+10}, LLL\text{11}, LZJ\text{+11}, PMG\textsuperscript{+16}, YS13, ZLLL12, LZL\textsuperscript{+15}, MKH15, XhD\text{15}, ZWY\textsuperscript{10}]. Branch [Ish10]. branching [BEL\textsuperscript{+11}, OZ\text{LSBH12}, STM17]. BrBr [LGW12]. Breaking [HRID16, SRR\text{16}, WWW\text{W18}]. bridge [CVG\text{14}, PH15]. bridged [KGR\textsuperscript{+16}, ZLZ\text{14}, ZLY\textsuperscript{+16}, ZZWX11]. bridges [MLY\textsuperscript{+13}, PH15]. Bridging [YLP\text{11}, dCD\text{P15}, LJJ\text{+11}, MIS\textsuperscript{+15}, BPC\text{13}]. Bringing [RR\text{11}]. broad [TZ12]. bromide [MG\text{15}]. bromination [SGS\textsuperscript{+16}]. Bromine [LWL\text{16}]. BR\text{OMOC} [DMN\text{15}]. Brooker [TYN\text{15}, TKYN\text{17}]. Brooks [HIS\text{17}]. Brownian [DZ\text{T11}, LJR\text{+12}]. brushes [DQ\text{16}]. btmgp [RHT\textsuperscript{+15}]. buck [KPF\textsuperscript{+15}]. Buckybowls [HVS\text{16}, CCCL\text{RO14}]. buffered [MJG\text{15}]. build [APK\text{14}]. builder [KOY\text{+12}, GS12, WCJ\text{+14}]. Building [MB14, CB\text{P14}, GS12, KSW16, MJBM12, RLG14, Tak11, TJB\text{12}, VVY\text{17}]. building-up [Tak11]. build-up [SS\text{13a}]. built [FC\text{PJM14}, KOP\text{+14}]. bulk [BC13, Man13, MBC13, NNS15, PAK15, QZ\text{10}b, RRC\textsuperscript{+15}, VBB\text{13a}, VVB\text{13}]. bulky [SL\text{C17}]. butadiene [MCC\text{11}]. butane [WK\text{C11}]. butane-like [WK\text{C11}]. butanol [BS\text{10}]. Butene [CS\text{M16}, MS\text{BF16}, W\text{vRSM14}]. butterfly [NDG\text{14}]. butyl [MG\text{15}]. butylbenzene [HCB\text{11}]. BX [YKH15].

C [Ld\text{SRR16}, LAH\text{S16}, LDL\text{17}, LC\text{WW10}, LWD\text{13}, MLQ\textsuperscript{+12}, MK\text{C17\text{a}, MCK17\text{b}, PS\text{G16}, RLA\text{+11}, SK\text{MS13}, STS\text{+10}, SBW12, Tak11, UT15, WC\text{y\textsuperscript{+11}, WWKS\text{16}, YZZ\textsuperscript{+17}, ZYG\textsuperscript{+14}, ZLY\textsuperscript{+16}, BS16\text{a}, VAMS\text{14}, Ben17, B\text{WKW10}\text{a, BS16}, BH13, CG12, ED15, FL15, GWT\textsuperscript{+17}, GMSV\text{14}, GZ\text{Z12}, HJ13, HVS\text{16, IMK\text{+16}, JLS\textsuperscript{+10}, KV14, KP10, LFB\text{14, LLC\text{17}, LDH\text{+14}, MSV\text{16}, MH11, Niz13, OPR16, PTK\text{11, Pie14, PZ\text{BA13}, RWR\text{+13}, SND\text{K16, TF\text{Q\text{+10}, TF\text{Q\text{+11, TS\text{15a, VAR\text{12, VED\text{10, WKC\text{10a, WL\text{W\text{+10, WS\text{10, WL\text{14, W\text{TH\text{+16, Yes\text{12, Yes\text{15, YDGZ15}]}]. C-termi

C2


Calculating [PNI13, SK12, WNP+16, WWD14, CPK12, EFS16, EPD+11, HAI+16, OK16, SM16a, WYT17, dRBO13]. Calculation [Fer13b, Fer13a, KSH13, MMJ10, MS15, SH11b, SOD+11, SOvG12, AC11a, Bac12, BW11a, BK17b, BD11, BL12, CHG+16, CG15, CX10, DKE+17, DSX+11, FD14, FGM11, GREA11, GCW16, Han11, JIS13, KNHN16, KN17, KB16, KDB13, LFN+10, LLW12, LZW+11, MYT+14, MLC13, MS12, NYN17, NFPD13, PDMT10, PAK15, Pie14, PW12, ROI4b, RZ16, RB12, RRK16, SBV10, SLIB12, SCSW13, SACdG14, SMM17, SR11, UT15, VVV+15a, VVG11, WCY+11, ZLL12, HH10].

Calculations [HBI+17, AR10, AAC+16, BE12, BLL13, BS10a, BTMS12, BH15, Bou14, BG12, BLZ+13, CR14, CCJC10, CS17, CCKK16, CMvG10, CXS10, CHKR10, DCH+11, EFAC13, EK17, EWK+13, EP12, EB12, EBK13, FAA15, FE14, GRAR0+14, GMO16, HASR+12, HYL+11, HS14a, HB14, HSH15, Hei13, HG10, HG13, HBL12, HYUS11, Ibr17, JCG+11, KK17a, KB10, KNN11, KGHK12, KKR+13, KERY+16, KCPMG12, KKL+13, KSH+17, LED0LdV17, LMZ11a, LCH10, LYC+13, LCA17, LvG13b, LCM+14, Lun12, MK17, MCLD10, MCK17a, MCK17b, NJ1+17, OHL12, OOT15, OZLSBH12, PBLdS12, PTK11, PHK14, POB13, PBBP11, PDG+16, PN13, PGW+17, RAR+11, RHT+15, RLD12, RR11, REV+17, RI01, RK15, SH15, SRSLO15, SP13, SSI16b, SCW11, SWPR11, SRS14, SMP17b, SMDS13, SH17, STT11, TLDG+12, TS10a].


[HRB$^+_{17}$, ZSB$^+_{16}$]. cavities/vacancies [HRB$^+_{17}$]. cavity [ZWS$^+_{10}$].
CAVS [SDZ17]. CB [BTMS12, CC18a, ILKR11]. CBS [KG15]. CBS-QB3 [KG15].
CC [Gii11, LLTC12]. CC2 [SGWA17]. CC3 [LZ14]. ccCA [RJWW12].
CCSD [BBI$^+_{11}$, CSLOA17, Gii11, KK17a, KKL$^+_{13}$, MVKS10, OPR16, PIC14, RS13, SRR16, SB14, YJ17].
Cc [SLIB12]. CDOCKER [GLB16]. C == [CROB16]. Cc [Ibr17, YOPB16].
cefotaxime [MFM$^+_{12}$].
cell [ACS12, CGBK13, Elk16, Fom11, Gon12, JMS14, SRL$^+_{15}$, VÀA14, dACP12].
Cells [FPV13, ACS12, DZA11, DGL$^+_{13}$, JYS$^+_{12}$, LZZ15a, SV11, SLC$^+_{17}$, TZ12, YJN$^+_{11}$].
cellular [VBD11].
Cellulose-Builder [GS12].
cementite [VED10].
cementite-type [VED10].
cementitious [TZ11].
CENSALC [SDMS13]. census [PPUBGD10].
center [IF$^+_{10}$, LRER13, YLL11, Yu12b]. centered [VI17]. centers [Gav12, WC14].
central [DGL$^+_{13}$, Yu12a].
centrality [RNVP13].
centric [LABSG17].
CEPA [Sch12, SB14].
ceramics [RKB$^+_{14}$]. cerium [SRL$^+_{15}$].
CF [JCG$^+_{10}$, NMLD13, RVdMB16, ZLL12, AR10, CROB16, NMLD13, ZZL$^+_{10a}$].
CFCF [NMLD13].
CH [AR10, LWD13, LJG$^+_{11}$, OZLSBH12, TLdG$^+_{12}$, WHZ12, ZZL$^+_{10b}$, ZYLL12, ZLL12, BS16b, CK10, CXW14, GY12, HVS16, JCG$^+_{10}$, KBC12, LW12, LGW12, LLTC12, LJG$^+_{11}$, MCU15, OOK11, RVCFF13, TCPPC14, VY17, VDVR14, WHZ12, ZZL$^+_{10a}$, DR11].
CHA/ [OOK11].
chaff [NMF$^+_{14}$]. Chain [vRWGS17, BFH$^+_{13}$, CHKR10, HAL14, KV14, KLS10, KMLS10, LPS$^+_{13}$, LZGS11, LP11b, LvG13a, LZLMP16, OZ14, PD12, PS10, QZM11, SA13, SISK10, SZBM13, TSN16]. chains [AFSW16, FP17a, JSW10, LZZ14, NPP13, Pla11, PLH16, TLdG$^+_{12}$, TS15b].
chalcogenides [SPS$^+_{12}$]. chalcone [CPLL11, YZ17].
challenge [SDM$^+_{16}$].
Challenges [HGY15, KHWB17, HLvdV13].
challenging [CAP17, VT14, WLF11].
change [EMD17].
changes [GDV17, GBS$^+_{17}$, HB15, LI13, MSL14, MO17, RO14b, YZGS14b].
Changing [XVN17, LLvG10]. channel [HYV13, PVL$^+_{13}$, SFBT17, SY16b, TCX$^+_{13}$]. channels [KC13a, LL10c, OKIS17]. character [BMB13, Cas14, Ibr17, RJJ$^+_{11}$, YSSB12]. characteristics [DPSL16, Gav12, LT14, Mat14, RDT14, TZ11]. Characterization [VT14, XWSW13, CBP$^+_{15}$, DGL$^+_{13}$, GBW$^+_{14}$, GZD12, Kop15b, MJBM12, MPA10, RNP13, ZYG$^+_{14}$].
Characterizing [LH11, PRSG13, Shf12, Yu12b]. characters [LSH$^+_{11}$, ZZL$^+_{10}$]. Charge [CMF$^+_{17}$, JM11, RDT14, SFDE16, AS15b, ANH$^+_{11}$, ALH$^+_{10}$, BCSCJ$^+_{13}$, BE16, CS14, CBTZ16, CMS13, Cor17, DS12a, DWR17, DADGR15, EFAC13, ENKK$^+_{17}$, GMG$^+_{10}$, HLWD15, JCGVPHT17, JZZM14, Kan15, KVR10, LLL11, LPE$^+_{10}$, LBDP12, MSV16, MHRR11, MPBJ11, NN18, OWB12, PL14, PTB$^+_{15}$, RO14b, Ric16, REL17, SPS$^+_{12}$, SSGS15, SMP17a, SFLG$^+_{17}$, SLC$^+_{17}$, TN10, TKNN10, UT15, VPR10, VAR12, VL17b, WCT$^+_{11}$, WWCL15, YKO$^+_{11}$, YWZ14, YLZ$^+_{10}$, YJ17, ZDZM13, dLC17].
charge-assisted [SSGS15]. charge-inverted [UT15, YJ17].
Charles [HS17]. CHARMM [MSK12, AKMYB18, BF17, DPNM11, GLB16, GZM11, HBJ17, HC14, JCL17, KLJ17, KYB13, LZdIL10, MSK10, MMZW14, RR14, VHA10, WCJ14, XVA16, YHVM12].
CHARMM-based [MMZW14]. CHARMM-compatible [KYB13].
CHARMM-GUI [HBJ17, KLJ17]. CHARMM27 [ST11].
CHARMM36 [HM13]. CHATT [Bac12].
CHClCH [WLHZ12]. CHEAP [MVKS10]. CHEAP-path [SA13]. CHEAP [HIS17].
CHEM [ABB13, CHR12b, HNWF12, ICS13, Kne11b, MSK12, RK16a, SFCCK15, SMM15a, GCC14, GKV13].
CHEMICAL [BLG10, BCP10, JCGVPHT17, OM12, SLLL13, VGL16, ALK15, ASS17, AAC16, APA14, Bac12, Ben17, Bou14, Cam15, CHP11, DKE17, DS12a, DI11, DB12, EOA11, FB10, FVB10, GH10, GGM12, GPMSM11, GPGSM12, HPT16b, HHDIC16, HJ13, Ihl12, JKS16, KV12, KASH14, KP11, LK11, LZH11, Li14a, Li14b, MDTD13, MDTD16, MN15, MAPB10, MSV12, MSSP17, MFR11, MMJ10, MH10, NCV10, NC13, NC14, OKS17, OSH17, ONTTL16, OC14, PTK11, PGO16, POG17, RK15, RSKG14, SRA17, SLT14, SCHO13, SEF16, SKMS13, SHB17, TLA10, TG12b, TR12, UD12, VBA13, WBT10, WCT11, WF16, Wei12b, WL14, Wu10, WDP12, YZ15a, YB16, ZY14, ZBB16, ZT14, dCDP15, VBD11, Chui10].
CHEMICAL-BONDING [MDTD13]. CHEMICALLY [EFAC13, ZZ12, Zim13].
CISPLATIN
Clarifying [RML+15], class [DWL11, HHWL17, ZLW10], classical
[DKJ10, CICH [RvdMB16], CICI [LGW12], clean [YR13], click [TKXT13], close [BLZ+13, MK17, RS13], Clos [YR13].
Closed [CYI+10, MA16, MS12, WWD14]. Closed-shell [MA16, WWD14]. Closo [HJ13]. Closo-carboranes [HJ13].
CM3 [VSA11]. CN [TS15b, YKH15, STS+10, TCPPC14, WHDL11]. CNO [OKIS17]. cNOR [BS16a]. CO
[BAC12, BPLL12, FD16, SC17, SSX+14, YXX17, ZBB16, Spr10, WVKS16, BPLL12, CCJ10, DHE+12, GLZ17, HF10, HVS16, HD10, LLC17, LPLB16, MG15, MBFG15, SKT11, WC13, CMM18, HYL+11, JCG+11, WJX+10]. coadsorbed [LLTIC12]. Coarse [MSL10, SNT14, BIP15, BLK12, CAD16, GMPB12, HHWL17, JCN16, KCK+17, KVQc+11, KLS10, KML10, L212, LZX16, LZZ14, LZLMP16, MBC11, MBC13, ML14, RSG+10, SLX+15, SDZ17, SOM+13, SJ17, SM15, SavG15, WBF17]. Coarse-grained [MSL10, SNT14, BLK12, CAD16, HHWL17, JCN16, KCK+17, KVQc+11, KLS10, KML10, L212, LZX16, LZZ14, LZLMP16, MBC11, MBC13, RSG+10, SLX+15, SDZ17, SJ17, SM15, SavG15]. coarse-graining [BIP15, GMPB12]. cobalamin [AALCM11]. cobalamin-dependent [AALCM11]. Code
[REL+14, BT10, GHK12, GP12, LLH14, LCPS13, RHR14, WK+10b, VV11]. codes [KSH+17, RGN10]. coding [QLQ11, YS10]. coefficient [FSD+18, WH11, WF16]. coefficients
Computing
[Ano10a, GKI15a, HDL+17, HRH+17, KHWB17, PBDW11, SN10, ACD+13a, ACD+13b, BK13, BZB+13, CHC+13, CKKK16, GM17, LPLA13, MK13a, MKO+13, OV14, OPB+12, Rod13, TF15, XYX17, Yan14, ZWL13].
concatenated [PSP15].
connected [PAA11]. concept [GRL+11, GRL+12, dSvD+16].
concerted [II10].
connection [Luc14].
considerable [LLD17].
Consideration [Fom11].
Consistent [CSEMB+16].
Consistently [IM17].
considerable [LLD17].
constant [AB16a, CS14, KSK11, KNP+12, MK17, PS13, RAGLL11, STM17, Vor12, WOH16, dACP12].
constant-distance [dACP12].
constants [AAMD+11, CBH14, CPK12, DSD+11, ECZWD17, FD14, GAI13, GKR13,
Constrained [SLG15, GRE11, GA12, VB13b, WBN+13], constraints [KB11a, OPBR17, OZS+13]. construct [HH10], constructed [HDL+17, ZLY+16]. Constructing [Che17, HS16b, LG11, SWA13].

construction [AGR11b, JCPC11, KSR17, LZX16, UIW+10, WWD14, YD17].


Continuous [Dry14, LPLA13, PZBA13, FGM11, LBGS16]. Continuum [JJJ16, Cam15, CY11, HZSS17, ISO+13, LFN+10, MUC15, SK12, SK17, TNG+10, WC13, WRHF10, XZ11]. contraction [HSN14, STM17]. contractions [KK17a]. Contrasting [TS15a], contribution [Pro16]. Contributions [JJH+13, ARRC15, BCNH+11, CGR16, CPN+17, ENKK+17, WS10].

control [BVY+12, DPAB16, Hel13, HH16b, LPLB16, SR10, XYW+14, ZQ14], controlled [VGTL16]. Controlling [FWB14].


Cooperativity [RS14, AFWS16, JSW10, SM16a]. coordinate [AMGB10, HSN14, Hel13, LL15, LL13a, MS10, WBN+13]. coordinates [BK15, LWK+14, NCV10, PH10a, Sch13, VB13b, You10, ZT14].

coordination [ASMS10, CRC13, HS16b, KJ10, Mor15]. copper [JRSHP14, KKPT11, SBC+11, SPR+13, WC14, AMSS10, CPK12, HRJ+14, HGHP14, HRJ+15, XWSW13]. coprocessors [WS13]. Copyright [Ano16-94, Ano16-95, Ano16-96, Ano16-97, Ano16-98, Ano16-99, Ano16-100, Ano16-101, Ano16-102, Ano16-90, Ano16-91, Ano16-92, Ano16-93].

KSH13, KSSH13, MMS16, Rui11, ST13, SPH11, STS15. correction
[HGHP14, NLP+16, RR12, SMGB11]. corrections
[JKS+16, KB10, KLN12, LCM+14, MGWR12, PTK11, RJPB12, RRK16,
SJZ+15, SSA+17, TG12a, VL17a]. correctly [ASMS10]. correlate
[MJLV14a]. correlated [BWKW10a, BWKW10b, EWK+13, KSH+17,
LLM11, MP11, yOTn16, RRK16, SM17, Vy16]. correlating [SNKS10].
Correlation [ASL+11, CKH17, SN16b, Vy16, CSKH15, CSKH16, ESM+12,
FRSA14, H13, HGCCGR+16, HG10, KSH13, KNP+12, LBH+11, MKGA10,
NYH+17, OAN15a, PTB+15, SPH11, VL17a, ZPP+16]. correlations
[CSKH16, SB10, TTB+10]. corresponding [PG14, RvL11]. Corrigendum
[Ano15-58, Fra16, HHT+13a, HRJ+15, HvM17, SSB13, WHAS+16].
COSMO [DS12a]. COSMO-RS [DS12a]. COSMOmic [JIS13]. Cost
[PDG+16, BLDK+13, BYE+16, CBP14, Gi11, LCM+14, SRR16, TF15].
cost-effective [LCM+14]. cost-efficient [CBP14]. Could
[EPH+13, EPH+15, TLA10]. Coulomb [FED17, IO13a, JKS+16, LMR14].
coulnic [DPAB16]. coumaric [HNN+17]. coumarin [MS11, ZDX11].
count [KTK17]. Counterpoise [SMGB11, LCM+14]. Counting
[QZ10a, RNP13]. couple [IYK11, Tsi17]. Coupled [DAB16, H614, VV14,
ACD+13a, ACD+13b, BYE+16, CAT+13, FZY+12, HDM+15, HGCCGR+16,
ILKR11, IYK11, JLIH+14, MC12, PGS+15, RKDM14, SB14, SH18, SM17].
Coupled-cluster [H614, VV14, BYE+16, HGCCGR+16, MC12, PGS+15].
coupled-cluster/Kohn [VV14]. coupled-electron [SB14]. coupling
[AMQ+14, BLZ+13, FD16, GP11a, KSK11, KNP+12, Kos16, LLB+12,
LSH+11, LWD13, MG11, PS17, Rui11, RRK16, SACdG14, Wu10, YB11,
ZTH+15, ZLZ14, ZYyIZ14]. couplings
[CSEMB+16, LK11, LZH+11, dVAG16]. covalency [HS14a]. Covalent
[WB10, FCCP17, HAI+16, KAR12, MR17, OZS+13, RS13, SFA17].
CovalentDock [OZS+13]. covalently [CZNA11]. Cover
[Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h,
Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano12o, Ano12p,
Ano12q, Ano12r, Ano12s, Ano12t, Ano13a, Ano13b, Ano13c, Ano13d,
Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13k, Ano13m,
Ano13n, Ano13o, Ano13p, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u,
Ano13v, Ano13x, Ano13y, Ano13z, Ano13w, Ano13z, Ano13-27, Ano13-28,
Ano13-29, Ano13-30, Ano13-31, Ano13b, Ano13c, Ano13d, Ano13e,
Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13k, Ano13m, Ano13n,
Ano13o, Ano13p, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v,
Ano13w, Ano13x, Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29,
Ano13-30, Ano13-31, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g,
Ano13h, Ano13i, Ano13j, Ano13k, Ano13m, Ano13n, Ano13o, Ano13p,
Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13x,
Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31,

density-density [SS16a], density-fitting [Hil13], Density-functional [Oht16, CHG+16, HNWF07, HNWF12, IM17, JCP14, KZZ+16, MFR+17, NF17, NN18, NO16, NNK+16, RHPWS13, SPSS+12, VED10]. density-peaks [LZS+17].

density-based [LZS+17].

density-density [SS16a]. density-fitting [Hil13]. Density-functional [Oht16, CHG+16, HNWF07, HNWF12, IM17, JCP14, KZZ+16, MFR+17, NF17, NN18, NO16, NNK+16, RHPWS13, SPSS+12, VED10]. density-peaks [LZS+17].

dependence [SMM+18]. dependency [DKT13, PHDH13]. dependent [AALCM11, BS16a, CHG+16, CP15, CKP10, DP15, EP+10, GTK10, HNWF07, HNWF12, HG10, HYUS11, JYS+12, KCPMG12, LPLS16, LZ12, LZGS11, Mat10, NS10, PAK17, PPJ14, PVJ10, RHPWS13, REL17, SY16a, SFBT17, Vik11, WHL+10, WHX+10, YLZ+10, ZXS+10, ZDX11].

determination [SE14]. derivation [SCMA+17, VVV+15]. derivative [MY17b, TPL+10].

Derivatives [KTSW11, CWHH11, CZH12, CBTZ16, CROB16, HSZ+11, JS17a, JYS+12, KG11, KPL15, LWGZ15, LWGW12, MFR+11, MS+15, NS10, PC14, RVB+12, RFN15, REH13, SBR13, SXZ13a, SXZ13b, VVJ15, VSD10, WGL+11, WRG+17, WDP+12, ZsA10, ZWZ11, ZZ12, ZZWX11].

derive [RVP+11]. derived [CIKT13, GMMH+16, KSR+16, LZGS11, MCLD10, OSS10, PLZ17, REL17, SOYC12, SE14, TBSM12]. Deriving [CCYL11].

descent [MS16]. describe [RHRCH16, RS13]. described [BM12, CCB15, KDS17].

describing [MKGA10, JCP14, JBSQG11, MY17b, VBD11].

descriptors [FCL+10, FZL+15, GJMMPAM+14, MH10, NK16, PKIC11, RB13b, TT+10, We12b, YLXC10, Yapr11, YDx16, ZXW16].

described [BM12, CCB15, KDS17]. Describing [MKGA10, JCP14, JBSQG11, MY17b, VBD11]. Description [FD16, MR17, BD12, BE16, Cam15, CRZ+18, LZLC13, MFR+11, PM13, PLH16, PVAM16, SRF+17, SSA+17, TKNN10, WvRSM14, WL14].

descriptor [DFF+15, MA16, PRYI+17, TMJ15, WMW+10, Yap11].

descriptor-based [DFF+15]. descriptors [FCL+10, FZL+15, GJMMPAM+14, MH10, NK16, PKIC11, RB13b, TT+10, We12b, YLXC10, Yapr11, YDx16, ZXW16]. Design [LCM16, Tak14, Tz12, VBD11, AM10, AFR17, BAM13, BEPM14, BPC13, CBP14, DPB+12, DPOS16, DGL+13, GS14, GMZ12, HHBY10, ISP+10, KSD+12, LABSG17, LBS10, MS16, PC11, SYDS11, SGM+13, St15, TKXT13, TRA+16, VVY17, VMPS15, XHLH16, ZSB+11, ZWP11, ZYW+16, ZWS+10].

designed [BLL13]. Designing [PsPE+10, ZA15, Fel10]. desolvation [BK17a]. detailed [ABB+12, ABB+13, GPC+16, MP13, MO15, MC10].

details [MBA14, RSG+10]. detected [TCPPC14]. Detecting [DVVP14].

Detection [CBP+15, BV14, CLX+10, ZLM+15]. detectors [SK13].

developers [GKV+13]. Developing [CK17, DSK17, LPS+13].

Development

[GLB16, GMMH+16, LLJ12, MMB+17, MMZW14, RZG+13, RLD12, SC17, TNYN16, WPM+15, ZA15, CYX+15, GMASBF16, GCP+13, LPLA13, PZA15, PPM15, WDHZ13, YWZ14, ZsA10, ZSYH12, CRC13, VKC10, WCDM11].

developments [YWJ+16]. Deviation [CSAdOM17].

deviations [HDL+14, KG15].

devices [DJX+11b, DJX+11a].

dewar [Bac12].

DFT [CLFRO18, SIG+15, YJ17, ZZY+16, AALCM11, AR10, AF14, ASMS10, BTMS12, BIL10, BTB+11, CLFR018, CMM18, CCB15, CH10, cCVG+14, CX10, DJD12, EFAC13, FVP14, FPRSI4, GMASBF16, HSH15, HRJ+14, HRIJ+15, HBI+17, JRSHP14, KG15, Kar17, KT12, KKL+13, KM13, KP10, LEdOLdv17, LRBB12, LZL+10, LZHH11, LXZ+10, LSH+11, LYSS11, LZLC13, LH14a, LSLW14, LCM+14, MMS16, MTD16, MG15, Mat10, MS11, MVKS10, Mor15, MCK17a, MCK17b, NKJ16, NC12, NMLD13, PTK11, PPM15, WDHZ13, YWZ14, ZsA10, ZSYH12, CRC13, VKC10, WCDM11].

DFT-based [NKJ16, NC12]. DFT-derived [REL17].

DFT-MD [GMASBF16]. DFT-predicted [WKLC12].

DFT/MM [RN17]. DFT/TD [LXZ+10]. DFT/TD-DFT [LXZ+10].

DFT/TDDFT [MS11].

DFTB [SA10, FHT+15, MR17].

DFTB/MM [RN17].

DFTB3 [KGW15].

DGeCl [MCLD10].

DH [SGPJS+17]. DH2 [SBW12].

di-mannose [VM11].

di-tetrazine-tetroxide [MCAG+16].

diabetic [DHOG13].

diagnosis [PC11].

Diagnosis [MC12, TDKT10]. diagonal [BMBJ11, KTK17].

diagonalization [BKŠ+11, HKR+14]. diagonalization-free [BKŠ+11, HKR+14].

diagram [OV14, VED10, ZY14].

diagrammatic [WWD14, YD17].

diameter [AS15a, KGHK12].


dianion [DP11, GRD+10, YZGS14a].

diarylalkyl [NS10].

diarylalkyl-imidazole [NS10].

diarylalkyl-triazole [NS10].

Diarylbibenzofuranone [SFA17].

diaryl dichalcogenides [ZWGO16]. diastereoselectivity [AARP17].

Diatomic [ATM18, LS11b, Tsi14].

diatomic [TG12b].

diatomic [CPN+17].

dicarbide [Kop16].

dichloropentacene [ZYG+15].

dichroism [HNHR13, SB13, SB15].

Dickerson [IPAA11].

dicopper [RHPWS13].

diels [BJSI12, CC18a, FB14a, GNDA+12, LZH16, ORZ11, ST13, dSVD+16].

difference [LLH17, WL10, You16, ZRCC11].

difference-dedicated [ZRC11]. differences [BVC13, GO13, HDL+17, KHWB17, LGL11].

Different [PH15, BRGN12, Dill15, FZL+15, GO13, GR11, GFPSD17, GMPB12, Kar17, MCS11, MC12, MPA12, NMLD13, NOKJ16, RNHN10, Rao11, SLP+12, SIG+15, TSNC+17, UT15, ZR10].

Differential [HHT+13a, HHT+13b, CJL+13, MY17a, MY17b].

Diet

[CLS12, CC18a, FBA14a, GNDA+12, LZH16, ORZ11, ST13, dSVD+16].
diffuse [YCGA10]. diffusion
[CPV+12, CC12a, GC11, RSLS13, ZW17, WH11]. diffusional [MBR+15].
Diffusive [SM16b], digitized [YNH+17], dihedral
[CYG+15, OZ14, SZBM13, WES13, ZRL+15], dihedrals [LDH+14], dihydro
[RS17a], dihydrofolate [RKDM14], dihydrogen [PM13, UT14, WHX+10],
dihydrogen-bonded [UT14, WHX+10], dihydrogen/hydride [PM13].
dihydropyrido [YZ15b], dilmide [MCC11], diiode [AARP17].
diode-induced [AARP17], diketopyrrolopyrrole [HLWD15],
diketopyrrolopyrrole-based [HLWD15], dilanthanide [ZLZ14], dilute
[KVR10]. dimensional [BPLL12, KYT+17, KRSC12, KTO13, MB16, PJ13, SG10a, TYN15, TCTX+13, TKC+11, ZWX16].
dimensionless [MS10]. dimensions [CHC+13, HAL14, SRL+15].
Dimer [LWL+16, ARRC15, ANH+11, CBTP17, CBTZ16, FCL+10, FMNC11, KCB+12, LCB10, PD11, SKY+11, Tac17, WWKS16, YCGA10].
dimeric [PS14]. dimerization [DSD+11, KAR12, TLA10, WJX+10].
dimerization/oligomerization [KAR12].
dimers [BCNH+11, BWKW10a, BWKW10b, CLFRO18, CK10, JKS+16, LJW11a, LMI+14, PVS12, RS13, SZS16, VT14, Zha11].
Dimetallic [ZYG+14].
dimethyl [GC11, WLC12, ZSWL12]. dimethylaminoazobenzene [KP10].
dimethylaminophenyl [YLZ+10]. dimethylnitrosamine [FFA14].
dimyristoylphosphatidylcholine [ML14], dinitrophenol [MIS+15].
dinuclear [OSS10, QLYL10]. dioxane [GM17].
dioxetanone [RSLML12, dSdS12a, dSdS12b].
Dioxide [SC17, Kop17b, QZ10b].
dioxygen [DSM+11]. dioxygenase [DGH+11].
dipeptide [EJ13, IO3b]. dipeptides [DHF+11, RSL16].
diphenyl [GKR13, Ray13, RKG11].
diphenylalanine [KLN16].
dipotassium [KT12].
Dipolar [YZZ13, CSS17, LK11].
Dipole [GH16b, LIRL+16, ZBG11, AS15b, BLBG+13, DHOG13, GH16a, HBBK10, KCB+12, LLHW14, MNNK10a, MNNK10b, PC14, Yan11].
dipped [IN13].
Dirac [JKS+16]. diradical [YSSB12].
Direct [LZY12b, WAM17, FF11, FSSW17, JCG+10, RSB+13, Yu12a, LLHM16].
directed [CH14, HHBY10]. direction [PAK17]. direction-dependent
[PAK17].
directionality [WGD+16]. diruthenium [CRC13].
disaccharides [GMSV14].
disconnectivity [SOJ14].
discover [Hsu14].
Discovery [AKMT11, AK16, FMG12, HYYZ13, Ibr11, IGK16, PVJ10, Zim13].
Discrepancy [Yan11].
discrete [EJ13, MCUJ15, WAM17].
discretization [AD10, LLFH16]. discriminate [UCFR16].
Discriminating [FZL+15].
discrimination [YL13].
discriminative [KS12]. discussion [CDB10].
disjoint [BK13].
dismutase [GEP+14]. disorder [LLL+12].
Disordered [MYT18, GP12, LC16, LC17a, NDLW13, SJD+15, ZC14].
dispersion [AG12, BCNH+11, CLFRO18, eCVG+14, GEG11, Han11, Has14, HGHP14, ITIN15, KB10, KSS13, LCM+14, RJPB12, STS15, SSB11, SSB13, TG12a, WM17].
dispersion-corrected [CLFRO18].
Dispersive [TG12a, SDB+16].
disproportionation [DLP11].
dissected [FNS+11]. Dissecting [CLFRO18].
dissertation [BMFG16]. dissimilarity [HS17a]. dissipation
electromagnetic [SEM12]. Electron [BK11, Bar14, BLG11, BWKW10a, BWKW10b, CEB015, HS16a, HRMAL+13, HGCCGR+16, KGR+16, Pil17, WWU12, ACD+13a, ACD+13b, ABGDN12, BHB12, CDB10, CAA10, CWHH11, CTP13, DaGR15, ED15, EP12, ESM+12, EP15, FRSA14, FED17, FCJM14, GNDA+12, HSH15, HPT17, HEMCZE+14, HAP+12, HBL12, IYK11, Jan16, JBSQG11, KPL13, KTK17, KYG+15, LW16, uLhY11, LHO17, LY16, LLJ12, LP11c, MKGA10, MRB14, Mat14, MBFP15, MKH+13, MCK17a, NYH+17, NS17, PAK17, PGdO+16, PSC11, PS17, PN13, PTB+15, PHT17, PC16, Ras17, Rod13, REL17, RSKG14, SB14, SHB17, SGHL13, SK11, SSA+17, VECT12, VL17a, VI17, Vyb16, WLW+10, WMW11, YKH+10, YLL11, ZPP+16, ZGS+10].

electron-correlation [NYH+17].

electron-deficient [YLL11].
electron-hole [PTB+15].

Electron-pair [WWU12], electron-withdrawing [CWHH11].

Electronegativity [FCPJM14].

Electronic [AMQ+14, ASS10, DaGR15, GNDA+12, HLWD15, Ibr17, KYCL11, KKL+13, LLBO12, LS11b, MAPB10, NIIT15, PMC+17, RLA+11, TN12, TN10, TFQ+10, TS15b, VI17, WRM+12, YW12, ZRCC11, AR15, AK10, AC12, BLZ+13, DKE+17, DOHG13, EH13, EWK+13, EBPK17b, FB10, GTT10, GRARO+14, GWX+12, GZZ12, HASR+12, HS14a, HSB+11, Hua16, IIF+10, KKPT11, KSM17, KG11, Kop15b, Kos16, KP10, LGOM+15, LX11, LBTV11, LBTM12, LXZ+10, LSH+11, LLSW14, MC10, MA16, MCF10, Mat10, NC14, NFI+16, OLA15, PHK14, PTB+15, PVAM16, Py13, RCM+13a, RML+15, RR12, RR11, SFA17, SLP+12, SRS14, SB15, SKGB13, TFQ+11, TD10, TS15a, TNG+10, TS11, TG12b, VVP12, VHR16, VAR12, VBA13, VGKL+17, WGL+10, WGL12, WJC+13, WO15, WSGN11, WZK+13, YK13, ZJZM13, wZbZ11, ZBB16, dCDP15, dVAG16].

electronic [vSGP10].
electronically [BSL+16, LSH+11, LYSS11, RIJ+11, SFCC++14, SFCC++15, YB11].
electrons [RN17].
electrons [EKH14, WCY+11, WRG+17, Xhd15, YCGA10].
electrophilic [MA16].
electrophilicity [VB16].

Electrostatic

[CLA16, LP11b, MLZZ12, BCNH+11, BK13, CCC+11, CS14, CPK12, CB11c, DLSA14, GBL+11, HOK17, IO13a, KTN10, KYG+15, Lar11, LCA17, LCM16, Mat14, PVJ13, RB13b, TY10, VMRSH+17, YKO+11, YY16, YMP14, YZL+15, ZDM13, ZBP11, KG12].
electrostatics

[CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NLP+16, SDZ17, SWPR11, UH+11, XY17, YMP14].
element

[BCCO10, GPK+16, RMGB11, TG12b, TCX+13, XY17].
elementary

[LPLB16, Zim13].

Elements

[TNK13, BV14, CWZ10, HU13, JJJ16, LFB14, SK15a, TDKT10, Ts14, WS12, Xhd15].
elevation [HH10].

ELF [RSKG14].

EL1 [BWKW10a, BWKW10b].

ELIA [BWKW10a, BWKW10b].

elimination [SL10, dCDP15].

Elisabeth [Ihl12].

ellipsoidal

[DGB+13, LDG+15].

Elongation [OLA15, MKGA10, MKGA10].

Elongation-MP2 [MKGA10].

Elucidating [HNHR13, TDP+12].
Elucidation [CPLL11, TNYN16]. embedded [DSF17, GMG10, HSH15].
embedding [CCB15, ESM12, HH16a, HH17, Höf14, HOK17, KSR17, NOKJ16, RR12, SDF17, SS16b]. emerges [MNNK10a]. emission [LX11, MCLD10, PLP16, SGWA17, WDP12, ZLL10]. emitted [PE11].

Emphasis [RCM13b, PD11].

Employee [BA11, DLMH12, KLN12, CK17, KB10, LL11, MPBJ11, PTK11, RJPB12, SZBM13, SBvG14, TM16, ZRL15, ZM10]. employing [GP11b, MLCD11, TG12b].

enabled [Aou16, BK17c, KYG15, LL10a, SR11]. enables [KK17a, XHLH16].

enantioselectivity [OAN15b]. encapsulated [EOO16, STS15].


Energetic [JW12, CG15, MCAG16, PGB17, SLHW09, TPL10, YSRSS10, ZZXW11, ZYL12].

Energetics [SFM14, BFK17a, BMFG16, DSF17, GAJ17, HEM17, JJH13, KB13, MP13, MBC16, OCW15, SJ11, SNS16, SL17, SDB16, ST13, SFBT17]. energies [AF14, AS14, AG12, BW11a, BLF14, BVH17, BS16b, BE16, CHG16, ČMD13, CH10, CTP13, CBG16, DHO13, DMJ17, DHH11, DPO16, FGM11, Gill11, GP11a, Grl13, HAK10, HH10, HH11, HLW17, HHWL17, IKN13, KSH13, Kar17, KSM17, KJDB12, KB11b, KY13, LJW11a, LW11, LHHW24, LH14a, MCS11, MS13, MSÅ12, MBE16, MMR10, NWW17, NMF14, OBW12, yOTn16, OAN15a, ORS16, PGCT12, PPJ14, RLDJ17, RDDS10, RAR11, RO14b, RZ16, RR14, Rob13, RJS17, SRR16, SK12, SHL13, SOD11, STM15, SGWA17, TS14, TSN16, UD12, VVG13, VECT12, VM11, WBT10, WS10, WJS13, W12, WX12, YAS13, YMP14, ZZ14, dAlD15, dRBO13].

Energy [DK11, GS16, IIHY15, JCGVPHT17, LFN10, LPLB16, SN16b, SSGS15, SKGB13, WM12, AMGB10, AC11a, Aou10a, AK10, AKN16, BCSC13, BPM15, BRE16, BH15, BS16a, BRLS08, BRLS12, BACSC10, BG17, Bou14, BD11, BWMSM10, BB11b, BB11c, BG12, CL13a, CK10, CDN15, CLA16, CY09, CX10, CZY11, CY13, CH16, CSXZ17, Che17, CS17, CHR12b, CH12a, CPK10, CMV10, CPK12, CWZB10, DGH11, DWR17, DBG11, DS12b, DH14, DWC17, EV14, FMNC11, Fer17, FED17, FCOC12, FSSW17, FCCP17, FLML11, GS14, GS15, GHK12, GO13, GMO16, HDM15, HLM10, HH15, HG13, HYM16, HYUS11, HJKJJ13, HYD10, HDHL15a, HDH15b, HDHL15c, IMK16, ISN13, JCPC11, JMLL13, JZ12, JZMM14, JX10, KCB12, KTM16, KB10, KNHN16, KN17, KHW17, KB11a, KOP15a, KOP16, KOP17a, KOP17b, KLS10].

energy [KML10, KCL14, LMZ11a, LZ12, LYT13, LZZ14, LGL11, LP11b, LX11, LHG11, LSH11, LZY12b, LLSW14, LAW16, MCvdV13, MCC11, MK13b,
WHL$^{+10}$, WHX$^{+10}$, YD17, YYT12, LZZ$^{+10}$]. excited-states [LLBO12].

exciton [HRH$^{+17}$, LSH$^{+11}$]. EXcitonic [JCGM18, ZMMM12]. excluded [LWZ$^{+17}$, Yan14]. exhibited [RWR$^{+13}$]. Existence [BMB13, WD10].

Exothermic [LWL$^{+16}$]. expand [BK17c, Car14]. expanded [MLQ$^{+12}$, TSNC$^{+17}$, YSSB12]. Expanding [GMZ12]. expansion [HAGK10, HSN14, LYC$^{+13}$, LRER13, NF17, SS16a, SNS13]. expansions [LZGS11]. Expected [LWZ$^{+17}$, Yan14]. exhibited [RWR$^{+13}$]. Existence [BMB13, WD10].

Exothermic [LWL$^{+16}$]. expand [BK17c, Car14]. expanded [MLQ$^{+12}$, TSNC$^{+17}$, YSSB12]. Expanding [GMZ12]. expansion [HAGK10, HSN14, LYC$^{+13}$, LRER13, NF17, SS16a, SNS13]. expansions [LZGS11]. Expected [LWZ$^{+17}$, Yan14]. exhibited [RWR$^{+13}$]. Existence [BMB13, WD10].

Exothermic [LWL$^{+16}$]. expand [BK17c, Car14]. expanded [MLQ$^{+12}$, TSNC$^{+17}$, YSSB12]. Expanding [GMZ12]. expansion [HAGK10, HSN14, LYC$^{+13}$, LRER13, NF17, SS16a, SNS13]. expansions [LZGS11]. Expected [LWZ$^{+17}$, Yan14]. exhibited [RWR$^{+13}$]. Existence [BMB13, WD10].
YWZ14, YJXZ13, YPKB12, YHVM12, ZRL+15, ZL11, ZP13, ZM10, ZCGM11].
forcefields [CBP14]. ForceFit [WKC+10b]. forces [EPD+10, ELK16, HNWF07, HNWF12, IO13, RN17, SDB+16].
ForConX [LDB+17]. forest [WZ17].
formaldehyde [CYY+17, GNGCA10, YPvD13]. Formalism [MKGA10, SFCCK+14, SFCCK+15, SMM17a]. formamides [JSW10].
fractures [NASH15]. Fragment [GK15, IIF+10, CIKT13, DR11, FMG12, GWF11, GKV+13, HB14, KS13, KS15, LMZ11, LFN+10, MFR+17, NF17, OOT15, OOK11, RKGN10, VBV13, WCT+11, dLC17].
Fragmentation [EFB16]. fragmented [JSXH16]. fragments [CM16, Kos16, KSR17, Sax12].
fractures-rooted [CM16]. framework [BHF+13, EH13, GP11a, HPT17, JBB+11, KTN10, MKGA10, OM12, PHT17, RCM+13, RML+15, Rz16, SK15, SWB+12, WYD13].
Frameworks [LSD+10, PLZ17, VVV+15b]. francium [TH13]. Franck [CHC+13, MCLD10, MLCD11]. Free
[Bou14, CBG16, GS16, GO13, GOM16, MCvdV13, OCW+15, PZCL16, SISK10, AC11a, AN10a, AK10, AKN16, BK+11, BSL11, BH15, BS16a, BD11, BB11b, BB11c, BG12, CY09, CXY11, CY13, Che17, Cs17, CHR+12, CHR+12a, CMvG10, DMJ17, DGH+11, DHP+11, DPOS16, Fer17, GS15, GHK12, GJMMPAM+14, GR13, HSL12, HH10, HH11, HDK+12, HLW+17, HSL+17, HDM+15, HG13, HYUS11, HKR+14, HHWL17, IMK+16, JML13, JCX10, KHWB17, KB11a, KB11b, KBY13, LMZ11a, LGL11, LP11b, LW+16, MSC+10, MS13, Mau14, MSAK12, MBE16, MJOM13, OSR16, OK16, PGC+12, PBLDS12, PPB11, PPJ14, RLDD17, RDDS10, RAR+11, RO14b, RZ16, RR14, SM14a, SFR+11, SWPR11, SY11, SH11b, SOD+11, SOvG12, SN10, SMM15, SMM15b, SMM+18, TS11, VLB+10, VVG13, VM11, WSH10, WCT+11, WWW18, WG12, XTG+11, XVN17, YOMT14].
free [YAS13, Yan14, YHH+13, ZZ14, ZPF14, ZYW+10b, ZH12, ZVY+15, dRBO13, WLZ11, XYW+14]. Free-energy [GO13, GMO16, BH15, CY09, HDM+15, HYUS11, IMK+16, JCX10, MIOM13, OSR16, PBBP11].

free-software [GJMPAM+14]. Free-standing [TS11]. freely [CH16].

frences [LBH+11, LLH17, WX12]. frequency


frontier [MGS+16, TZ12]. frozen

[BVC13, Fer13b, Fer13a, HH16a, HH17, Hop14, SDF+17]. frozen-density [HH16a, HH17, Hop14, SDF+17]. fructose [RAR+11]. fructose-1 [RAR+11].

car [SV11]. Fukui [BVC13, PRY17, SBR13, YVEI+17]. Full

[STM17, ACD+13a, ACD+13b, BPLL12, PS17, TSC+13, dSDdAR10].

full-pivoting [PS17]. Fullerene [GKSS14, KCK+15, KP10, Oht16, TPL+10, TFO+11, TTB+10, XFTW15, YDGZ15, ZSL+11, ZZ12, SWA13].

fullerene-based [TTB+10]. fullerenes

[GZHi0, GLF16, MCK17a, MCK17b, SWA13, STS15, WTH+16]. Fullrnc

[Aou16]. Fully [AG12, ZST14, FBY+17, GBL+11, KG13, LZZ+13]. function

[ABDGNI12, AB16b, BLG11, CKP10, GS14, GND+12, GEG11, HH16a, HBL12, HMYZ16, JLCA17, JMS13, Kop15a, LL13a, LHL11, LCB10, LIRR+16, MB16, yOTn16, ON14, Pi17, PRY17, RZG+13, RL11, S16a, SFG+17, TCB16, TO10, UM13, UCFR16, WO15, WDHZ13, YVEI+17, ZLT13, vSGP10].

function-based [WDHZ13]. function-guided [YVEI+17]. Functional

[FPV13, AMK11, ALK+15, Aon15-59, AG12, ASS10, BY11, BLBG+13, BK17b, BZB+13, BG13, CHG+16, CRZ+18, CR14, CWHH11, CSKH15, CSKH16, CKH17, CSXZ17, CC11, CNK97, CPLL11, CB11d, FD16, GAI14, GHL17, GZL+12, GNGCA10, GSS13, GEG11, GAE+17, GWPJ11, HHi1, HDL+17, HNWF07, HNWF12, HPT17, HG10, HZSS17, INT18, IKN13, IM17, JCP14, JLF+14, JW16, JYS+12, KD10, KKPT11, KOP+14, KGHK12, KB13, KZG+16, KL12, LCW12, LBGS16, LGW12, LBTV11, LBTV12, LSH12, LH14b, LH17, LPMT17, MAK14, MWJ+11, MFR+17, Mor15, MMJ10, NF17, NN18, NO16, NN+16, Oht16, ORZ11, OM12, PA17, PPH+14, Pie14, PD11, QZ10b, JRPB12, RS13, RB12, RSLML12, RHPWS13, RHT+15, Rui11, SPF+12, SH15, SFG+17, SCW11, SBT17, SEF+16, SE14, SH14, ST13, SHL+13, SPH11, SMM15a].

functional

[SMM15b, SMM+18, SKTT11, SZSS16, STS15, TLdG+12, TG12a, TS10b, VV14, VIK11, VLL17a, VI17, VLGK+17, VED10, WKC10a, WHL+10, WCWW11, WDLG12, WYT17, WHX+10, WL14, WTH+16, WGN+16, XYYW+14, YJ11, YLZ+10, YS13, ZXS+10, ZWLX11, ZSL12, ZL14, ZDX11, ZYG+14, ZYW+10b, ZYW10a, ZLHH14, ZGS+10, dSdS12a, dSdS12b].

functional/basis [PD11]. functionalities [KAG+12].

functionalized [KYKR15, LdSR16]. functionals [Ben17, CCB15, CG16, DH17, DOM+11, DWC17, FPR14, HG10, HBI+17, KB10, KSH13, KSSH13, Kar17, KM13, LBH+11, LH14a, LKK16a, PW12, RSG14, Rui11, SGPJS+17, Sea10, SDM+16, SPR+13, SZX13a, SXX3b, WYT17, Yu12b, ZTH+15, dSDLBNB17].
functions of [BLZ+13, CD13, CC11, CVG14, Fer13b, Fer13a, FFA14, Fra15, Fra16, GSHM10, GZ14, KK17a, LRR13, MY17b, Mit13, MLCD11, PHT17, Pro16, RHCH16, SFM14, SYDS11, Sun15, TNYN16, WZ17, TKN13].

fundamental [CD16, XLYZ10]. furanosides [KRTB10]. Further [RTS+13, FVB10, PZA15], fused [CZY11], fusion [OLY17], Fuzzy [FPV13, SK12, SK17]. fuzzy-border [SK12, SK17]. FXeOxEF [ARLP13].


Garriga [Ihl12]. Garriga-Sust [Ihl12]. Gas [ATM18, ABB+12, PL17, ARLP13, DHE+12, GYX+10, JKS+16, KD10, LPK16, LJW11a, LPLB16, MP13, MFMI+12, NIIT15, PGS+15, PMG+16, PSCI11, RWR+13, Sea10, SYZ+17, STS15, YHG+11, ZSZ+14, ZYR+15, ZLHH14, ABB+13].


Gauss [MY17a]. Gauss-type [MY17a]. GAUSSIAN [RS+12, OYK+11, Bow14, DLL+10, EPD+10, JLC17, Leh15, MG11, MKB+13, POB13, SPH11, Sun15, TH13, VKTR15, ZKE+17].


Generalized [GH16b, KCPMG12, AB16b, BSPP+13, DSF17, FCE15, GH16a, LL10a, MA16, PS13, SZTSM10, SSBB14, VMP17, WWKS11, WHM10, WBVE16].


GenLocDip [GH16b]. GeO [DLSD13]. Geometric [MK11, CDB10, CDBM11, EH13, FXC+13, HHT+13a, HHT+13b, LFH16, REH13, TCC+13].

geometric-quantum [CDBM11]. Geometrical [DPAB16, HRJ+14, JRSHP14, LCM+14, SPR+13, Tak10, UT14, HRJ+15].
Geometrically. geometries
[Alg17, HCP15, SRA17, Tak10, LXZ+10]. Geometry
[MP13, BW11b, EPD+10, FB10, Kow11, LIRL+16, MCLD10, OZS+13,
Pon10, RS13, REH13, SLG15, SMM17, VBV13b, WAB17, WX12].
geometry-dependent [EPD+10]. Germanium [GSMM15, ALH+10].
GeSbTe [NIIT15]. GFP [UD12]. GGA [BG13, EH13]. ghost [CMF+17].
[HYYZ13]. gibberellin-binding [HYYZ13]. Gini [WF16]. GIST
[RNSF+16]. glass [GFGS18]. glasses [You10]. Global
[LvDH13, OKIS13, PRSG13, Tak10, BK17b, CPN+17, DS15, DMAH15,
Pon10, RS13, REH13, SLG15, VBV13b, WAB17, WX12].
glucopyranose [HH10]. glucosamine [ZBP11, ZP13]. Glucose [APY+
16]. GLYCAM06 [SA10]. GLYCAM06/TIP3P [SA10]. Glycan [JSD+
11]. glycine [DB12, DP15, FCD10, MC10]. glycoconjugate [LABSG17].
glycoproteins [JSD+11, PFVL14]. glycosaminoglycan [CHRKR10, SA10].
glycosidic [HH11]. glycosyltransferase [RN17]. GmbH [Spr10]. GMCT
[UU12]. GneimoSim [LWK+14]. gold
[Auo15-58, BHS14, CJC10, FHT+15, GAMAC+14, Li14a, Li14b, LHKS12,
LH14b, MFR+11, MG14, MBFG15, SRR16, SKRT11, YLL11].
gold-thiolates [FHT+15]. Goldberg [WTH+16]. Good [SB10].GPCR
[LLHM16, MF+17]. GPGBP [UM13]. GPR119 [HK18]. GPU [AKK+
16, AGB13, BK17c, CVT+11, DZT11, HAP+12, Kan15, KGHC15, KPF+
15, PZCL16, REV+17, SBV10, SOM+13, UTM11, YLGX14, YSG12, ZLL+
13]. GPU-accelerated [AGB13, CVT+11, HAP+12, YLGX14, ZLL+
13].
GPU-based [KGHC15]. GPU-enabled [BK17c]. GPUs
[GBL+11, HLW+17, KK17a, RSRR15]. Gradient
[DS15, CDM10, HBBY10, KN17, SH15]. gradient-directed [HBBY10].
Gradients [GP11a, WM12, BWMSM10, CB25, HH16a, HH17, LBGS16,
LFN+10, RS14, SFG+17, SSMW09, SLG15, vLBDR12]. grafting
[KKR+13]. grain [SOM+13]. grained
[BLKP12, CAD16, HHWL17, JC16, KCK+17, KVQC+11, KLS10, KMLE10,
LZ12, LZX16, LZZ14, LZLMP16, MSL10, MBC11, MBC13, NST14,
RSG+10, SLX+15, SDAZ17, SJ17, SM15, SAVG15, WBF17]. graining
[BJP15, GMPB12, ML14]. Grand [HLvdV13, PHH+12]. grand-canonical
[PHH+12]. Graph [WSH10, DH14, GPGSM11, GPGSM12, IHL12, MCM12,
PsDPE+10, Pog10, RPNP10]. graph-based [DH14]. Graph-theoretical
[WSH10, PsDPE+10, Pog10]. graphene [YZZ+17].
[CM18, dRCFGRB18, DJX+11b, DJX+11a, JWO15, LWZK13, LCM+14,
PL18, RRR14, SDF12, WCT+11, WSZW15, WYL+15, WTH+16, YSSB12,
YZZ+17]. graphitic [HASR+12]. graphical
[All11, GLB+11, HZY+10, LMLC11, LBB+15, PVZ13, SEF+16, STH+10,
WSGN11, WS13, YWJ+16, YDL+10, YN15, YS10, ZKE+17]. graphics
[AB16a, AB16b, BDTP11, CKKK16, EP10, HKR12, HEMCZE+14, MSSP17,
48

HYUS11, KOY12, KZK12, KV15b, OK16, TFQ10, TJB12, LZZ14.

hindrance [MP17a]. Hirshfeld
[Man13, VVB13, VGV11, EV14, GBVA11, OVKP15, VB13a].

Hirshfeld-based [OVKP15]. Hirshfeld-I
[Man13, VVB13, VGV11, VB13a]. histidine [KFY13, WC14].
histogram [Fer17, HHWL17, SH11b, ZH12]. histone
[GHK12, GH10, GSD10, KC13a]. HIV
[DL15, NHH16, OBW12, SY12, TT10, UNT16, XLY12, ZsA10]. HIV-1
[DL15, NHH16, SY12, TT10, UNT16, XLY12]. HIVg41
[AFBR17, BAMR13]. HIV-1
[DL15, NHN16, SYH12, TTB10, UNT16, XLY12].

HIVgp41 [AFBR17, BAMR13]. HMH
[LDJ10]. HNCN
[WHDL11]. HNO
[BLG10]. HOB
[ALC10]. hole
[Cas13, CWHH11, EPH13, GZZ15b, PAK17, PTB15].

Holliday [Ish10, She12]. holographic
[CDB10]. HolT
[She12]. HOMO
[RS17a]. Homocysteine
[AALCM11]. homologated [ZLL10].
homologation [GRCL12]. Homology
[ZX11, BPB11, DJ13, KOY12, XFTW15, YZ16]. homology-model
[KOY12]. homology/ab [DJ13]. homolysis [SZ17].

Homonuclear [BWKW10a, BWKW10b]. homopeptides [FCD10]. HomoSAR
[BPC13]. HONO
[BLG10]. HOONO
[BLG11]. hopping
[JLH14, KV14, LZW11, RDRC16, SRSLO15]. Horizontal
[PC16]. hormone [HYYZ13, LLL10, NS10, OME16]. hormone-dependent
[NS10]. hormone-receptor [OME16]. horsetail [MCRL17]. Host
[CC18b, OAN15b, YDGZ15]. hot [RFHG10]. Hou
[JW12]. HOX
[LZJ11]. HP
[KL10]. HP-36 [KL10]. HPe [dSDdAR10]. HSE
[VLGK17]. HSICl
[LX11]. HSiCl/DSiCl [LX11]. Hua
[JW12]. Hückel
[FL15, SKT11]. Huffman [QLQ11]. huge
[NNK16, OHPR17]. huisgen [ZZWT12]. human
[OME16, SLY10, ZX11]. hunter [CMF17, She12]. Huzinaga
[Fer13b]. HXeOXeF
[ARLP13]. HXeOXeH
[ARLP13]. Hybrid
[CRG16, KSI15, VVY17, ZDKM12, BTA13, BG13, CCB15, CBG17, CSKH15, CSX17, CC11, DR11, DJ13, FHT15, GFG11, HZSS17, JMS14, KKR13, KJM17, LHB11, LT14, MJS15, OK16, PW12, RSG14, SGPS17, Sea10, SZX13a, SZX13b, VI17, WNM17, ZWLN11, ZWLN13, HPT17]. hybrid-meta
[BG13]. hybrid-parallel
[KJM17]. hybridized
[DC13]. Hybridizing
[RDRC16, FZL15]. hybrids
[KM13]. hydratase
[LT13]. Hydrated
[ALH10, BMFG16, CGPP11, GBL11, GNGCA10, LPE10, LBDP12, VPR10]. hydrates
[LZLC13]. Hydration
[HL14, AS14, DQ16, KB11b, KYB13, OK16, PPO10, RZ16, SK12, SWPR11, WBT10, WC13, WG12].

Hydrazine
[GZL12]. hydrazo
[WDLG12]. hydrazo-1
[WDLG12]. hydrazone
[HPT16a, ZZWT12]. hydride
[RKDM14]. hydrides
[DM15, PGC12, RMGB11, WKC11]. hydricid
[Jab14]. hydroamination
[KT12]. hydroazidation
[YXZ17]. hydrobromic
[CYY17]. hydrocarbon
[CB11d, KSM16, Kar17, MH17, SV15, WDW12]. hydrocarbons
[PL18, SBvG14]. hydrocyanation
[HDB15]. hydrodynamic
[AKK16]. hydroformylation
[dSDdAR10]. Hydrogen
hydrogen-abstraction [GY12].

hydrogen-bond [TD11, BK17a, CD11].

hydrogen-bonded [B LFZ13, DKT13, JCP14, LJW11a, LHHW14, PAT+10, UT15, ZDX11].


hydrogen-bridged [ZLY+16]. hydrogen-contaminated [YR13].

hydrogen-Disordered [MYT18]. hydrogen-storage [BEM14].

hydrogen-transfer [ZW17]. hydrogenase [GS11].

hydrogenation [JJAB16]. hydrolase [BHNS14].

hydrolyses [YZGS14b]. hydrolysis [LHT15, MFMP+12, XZ11, YZGS14a].

hydroperoxyl [AAMD+11]. hydrophobic

hydrophobic/hydrophilic [PAK15]. hydrophobicity [CH14, SV15].

hydrostatic [FCW+14]. hydroxamate [GWZ15, GPdC+16].


hydroxyl [DPNM11, GKR13, JCG+10, KS13b, Ray13, RKG11, TTR+12, ZSZ+14].

hydroxylated [CCJ+11, SH14]. hydroxylation [TYL+12, VCM15].

hydroxylationts [MRR11]. hydroxymethyl [HH11].

hydroxyethylfurural [APY+16]. hydroxynaphthaldehyde [MPG11].

hydroxyphenylpyruvate [DGH+11]. hydroxysteroid [ZX11].

hydroxysulfanyl [TL16]. Hyper [FRN15, BLBG+13, BZB+13, RFN15].


HZSM [cCVG+14]. HZSM-5 [cCVG+14].
RLL$^+$10, DL16, JSD$^+$11, MPNS13, RLDJ17, WSH10, YZWC11, ZYvIZ14.

identifier [Ihl12]. identifiers [GPGSM11, GPGSM12]. identify [LLHM16, LHL$^+$10]. Identifying


Ano16l, Ano16m, Ano16n, Ano16o, Ano16p, Ano16q, Ano16r, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16-29, Ano16-30, Ano16-31, Ano16-32, Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16b, Ano16-39, Ano16-40, Ano16-41, Ano16c, Ano16s, Ano16t. Image [Ano16-37, Ano16-38, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano16-53, Ano16-54, Ano16-55, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano17a, Ano17b, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17m, Ano17n, Ano17o, Ano17p, Ano17r, Ano17s, Ano17u, Ano17v, Ano17w, Ano17x, Ano17y, Ano17z, Ano17-27, Ano17-28, Ano17-29, Ano17-30, Ano17-31, Ano17-32, Ano17-33, Ano17-34, Ano17b, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17m, Ano17n, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano18a, Ano18b, Ano18c, Ano18d, Ano18e, Ano18f, Cor17, LCM16, SFLG+17, YHH+13]. images [LLJ12, MBFP15]. imatinib [AS10]. imidazo [YLZ10]. Imidazole [FD16, LWGZ15, NS10, YKH+10]. Imidazolium [MG15]. imidogen [Kop15a]. imine [AS11, GG10, HDB15]. imino [GRCL12]. immediate [HTS17]. Impact [ABM+15, DPNM11, MCS11, vADC+14, JMML13, NW17]. Implementation [AMGB10, BMRI11, HKR+14, ITIN15, KB14b, KK17b, LRvdSM15, LPLA13, LBB+15, MHT+18, RJPB12, RSG14, SN16a, ZMMM12, AB16a, BTB+11, CHG+16, Cas13, CEBO15, CSSB11, EWK+13, KS13a, KNHN16, KMLS10, KWG15, LL10a, LLZA12, LMR14, MKGA10, MBR+15, MYT+14, NYH+17, NN18, OYK+11, RSR+12, REV+17, SZX13a, SZX13b, TKT11, WPM+15]. implementations [LSD+10]. implemented [BVHI17, DLSA14, SR10, VBV13b]. Implementing [SCOJ13]. Implications [CV12, VVY17, CBG16, LP11b, LTP11, RB12]. Implicit [BEM14, CAD16, Has14, CBG16, EK15, FBEM11, KJDB12, KB11a, KB11b, LC17b, ML14, SSBW14, SLX+15, SCMA+17, TCC+13, WWKS11, YL13]. implicit-solvent [WWKS11]. Importance [APA+14, CPK12, ENKK+17, NMF+14, OOK11, Ham11, KTN10, PBWD11, SDZ17, TNSS17, TKNN10]. important [AST+16, BZH14, MG11]. importing [FN12]. impregnated [GLZ17]. improve [CIKT13, DLL+10, DPSL16, Gon12, LLL+10, VB10]. Improved [BS16a, LRER13, CCM15, DPB+12, DSF17, GCCM15, KSR+16, MP11, RTP+13, RDR16, SSBW14, YS10]. improvement [GSHM10, NLP+16]. Improvements [JCX10, AB16b, LRBB12, BB11c]. improves [BBOB16]. Improving [DWL11, GS16, LN15, PLH16, SB14, SACdG14, SA11, WZ17, ZWX16, ZYS+10, GS15, GFPSD17, GZ14, FZY+12, TO10]. impurities [SBC+11]. IMSPeptider [dCLFGL13]. In/Si [LGKS17]. inactive [CV12]. include [PZA15]. includes [HBKL10]. including [KL14, SFLG+17, BL12, FAA15, FD16, LH14a, SPH11, TG12a, WC14, YB11]. inclusion [CGR16, LZ11]. Incorporating [LHO17, Yan14, CSKH16, GCCM15, ZBP11]. Incorporation [BTT10, DDP16]. incremental [DCS15, LTA+11]. increments [MS15]. independence [LC17a]. independent
indispensable

individual

indole

induce

Induced

induction

inefficient

Inequivalence

inexpensive

infantum

inguence

Informatics

Informatics-Based

Information

Informational

initialization

Inherent

inhibition

inhibitor

information-theoretic

informed

infrared

ingredients

Inh

Initio
Interactive [BRP+12, BGR13].

interactiveness [CQFC10].

interatomic [DPAB16, FCCP17, YKO+11, dLC17].

interconnections [GLF16].

interconversion [HH10].

Interdependence [WAB17].

interest [BCNH+11, OZLSBH12].

interface [Alli11, BDTP11, CSSB11, GRP+12, GCW14, HL14, JJW+14, KG13, LJR+12, LZdIL+10, LBB+15, MSSH17, OYK+11, PHH+12, PVZ13, RR14, RSR+12, SN16a, SYDS11, SISK10, STH+10, VKTR15, VLI7b, WPM+15, ZWL13].

interfaces [PGCT+12, RRF11, SSAS10].

interfacial [NFPD13].

Interfacing [MSvG12].

Interferometry [JAH+17].

intermediate [TDP+12].

Intermolecular [FMNC11, VECT12, Ano10a, BLF14, BLDK+13, CCLP12, KCL+14, LZY12b, LZLC13, RRH12, SN10, TY10, TNG+10, VVP12, WGD+16, ZL+12, ZLT13].

Internal [LL15, REH13, LWK+14, NCV10, PH10a, TNG+10, VLGK17, VBV13b, WBN+13].

Internal-to-Cartesian [REH13].

internally [SMP17b].

Internucleotide [LZH+11].

interoperability [REL+14].

interphase [BVY+12].

Interplay [FC16, LLL+11, YKH15, CCLCGR14].

interpretation [DCOD13, TLA10, WXL17, XFX+16].

Interpreting [CLA16].

interprotein [JZ12].

intersite [LLLM11].

interstitial [GM17].

intersystem [AMQ+14, QCR12].

intervalence [DAdGR15].

intervals [LL11].

intra [LZY12b].

intra- [LZY12b].

intraminimum [ABD11].

Intramolecular [DBG11, GWF11, KP10, MH17, CROB16, HB15, KFY+13, KV14, LWGZ15, LTP11, MMT14, MPSG11, SSB11, SSB13, VVJ15, YK13, YLZ+10, dALS+15, dLC17].

intraphase [BVY+12].

intrinsic [AMGB10, OVPK15].

intrinsicly [LC16].

Introducing [DJD12].

Introduction [HIS17, Sie15, SJ17].

intuitive [EFAC13].

invariant [CWZB10].

Inverse [KTT16, GD10, JMS13, WHK+12].

inversion [SP13, GG10].

invert [KZZ+16].

inverted [UT15, YJ17].

investigate [dSAdSL13].

investigated [SLY+10, SCW11, YS13].

Investigation [ALV+10, CAP17, GY10, PH10b, WS10, ZY14, AvKSP16, AMK11, ABB+12, ABB+13, CWT+12, CYY+17, CZH12, CH10, GDV17, HXM+16, KCB+12, KV15b, LLM11, LLB+12, LZY+12a, LLDF17, LZX+10, MLQ+12, MP13, OAN15b, PZA15, PVS12, QCR12, RDT14, RRC+15, SH14, Tak11, TPL+10, TS10b, TR12, VVP12, YJN+11, YU12a, ZZ10, ZZ11, ZSWL12, ZBMZH15].

investigations [GZL+12, KAR12, LWWG12, TSJ+10, WS12, YPvD13].

Invisible [SDM+16].

involving [ARLP13, GND+12, LEDOLd17, LRRR13, NFG+13, OSHG17, SLT14, SL+15, YZZ+17].

iodanes [SLT14].

iodine [ACS12, SLT14, SL+15, KLN12].

Ion [Fra15, Fra16, LZTV10, DMN15, DMN14, EK15, JAH+17, JLCA17, KTK17, KJ10, LEDOLd17, LJ+12, LPE+10, MMB+17, MH11, NC13, PGY15, PL14, RTS+13, SSGS15, SV11, TCX+13, VPR10, Wk11, WC14, ZZ10].
ion-associated [ZZ10]. Ion-exchanged [LZTV10]. ion-pairing [KTK17].
ionisation [CTP13]. ionization [ACD+13a, ACD+13b, BG17, CBG17, GWF11, LGOM+15, LK13, yOTa16, SSB+16, SGHL13, Tac17, VL17a]. ionizations [LGVA14]. ions [AS14, BDTP11, CCCLRo14, CC12a, EKH14, PRJ+17, PZa15, SNS16, SGH+16, WKC10a, XP13]. IP [BK17b]. IP-tuned [BK17b]. IPRO [PGL+15]. IQA [CSM16]. IR
[DCOD13, CWT+12, LWL+11, LXZ+10, WJX+10]. irGPU.proton.Net
[Kan15]. iridium [CWT+12, HDPM14, KB13]. Iridium-catalyzed [KB13].
iridium-containing [HDPM14]. Iron [HS14a, AKMYB18, BG13, CTR13, GBGR16, HS16b, KPL13, KPL15, MC10, SBC+11, TS10b, VBMA13, EH13].
iron-containing [AKMYB18]. iron-sulfur [CTR13, HS16b]. Irregular
Isolated [FL15]. Isomeric [FL15]. isomerism [RS17b]. Isomerization
[BW11b, DBGO+17, EFB16, BLG10, BMFG16, MSBF16, OKIS17, SJD11, Su10, WCL+11, ZWZ11]. Isomers
[CSM16, ZWZ11, Kar17, OKIS17, WCL+11]. isotope
[KTT16, MRK11, NASH15, ORZ11, UT14, UT15, VKAM12, WXY14].
isotope-substituted [UT14]. isotopomers [UT14]. isotropic
Joswig [Spr10]. Journal [Ano15-59, Ano10b, GS16, MFEM16, XFG+16]. judging [RCM+13b]. Jumping [MS17], junction [Ish10], junctions [LZW+11]

Less [SA10].  Letters
[BCJC+14, Cor17, GKR13, GPGSM12, Ihl12, JW12, KR14, Man13, Ray13, RSLML12, SFLG+17, VVB13, WM12, dSDS12b, vLBBR12].  LEUS [BH15].
level [BVHH17, DMJ17, EWK+13, FFA14, HJKJ13, JCG+10, KSM16, KSM17, KKN11, MSC+10, MCLD10, OSR16, PVL+13, PTK11, PML+12, PB14, VAMS14, WWD14, ZM3M12].  levels
[AC12, BCSCJ+13, BY11, BACSCJ+10, HY12, Hua16, KHW17, Kop15a, Kop16, Kop17a, Kop17b, MK13b, dSAdSL13].  leveraged [EPH+15].  Lewis
[EHSPT16, KASH14, Li14].  Li
[DDM+15, JW12, RL+11, YCGA10, YHCS11, BWKW10a, RL+11, YCGA10, SBW12].  Libcint [Sun15].
LIBEFP [KS13a, KS15].  libKEDF [DWC17].  Libra [Aki16].  libraries
[LG11, RLL+10, WF16].  Library
[KSD+12, Aki16, DWW17, EWK+13, FRN15, KSL13a, KSL15, LRvE17, LMMZ11a, LAS+14, MZZ11, SC11, VAR12, Yes12, Yes15].  library-based [MZZ11].
LICHEM [KL+16].  LiCN [LLL+11].  LIE
[CZY11, VLB+10].  life [RHT+15].  lifetimes [CH10].  Ligand
[DPOS16, KC13a, MNNK10a, VCC10, AB11, BKLA13, BPB11, BCG10, BBG+18, BS10c, CM13, CTK13, CHR+12b, CHR+12a, DFF+15, FTLF12, FBMM11, FRLN10, GHIK12, GDV17, GS11, GZ14, HIR12, HG13, KL+17, KL14, KVB13, KTO11, KN11, LL+10, LWL+11, LBS10, MC10, MGWR12, MG14, MFR+17, NST14, NFG+13, NMF+14, OBW12, OHNK11, OGL10, OSR16, OCLM14, OOT15, PGCT+12, PK17, PP14, PV+11, RLDJ17, RZG+13, RCR+16, RVP11, RVP+11, S+18, SL+18, SKKS13, STM+15, TLY+12, TNSS17, VVG13, VOR10, WDVN12, WNP+16, WZ17, YZ16, dRBO13, YZZ16, SCH+11].  ligand-based [RVP+11].
ligand-binding [GDV17, MGWR12, OSR16, RVP11b].  ligand-field
[BBG+18].  ligand-induced [KL14].  ligand-receptor [FRLN10, VCC10].
ligand-sized [OGL10].  ligands
[CS17, GPDC+16, HRC13, LL10, LZC+10, LS11b, SSP+13, TS10b, ZRCC12, ZWY+10b].  ligated [EH13, WC14].
LigDockCSA [SHL+11].  light
[HXM+16, PE11, REL17].  light-driven
[HXM+16, REL17].  lighter [WD10].  Lightweight [RLG14].  like
[AASP18, Che17, EPH+15, KOY+12, KB14b, MP17b, OAN15b, SDF+17, SM15, UCFR16, VHA+10, WKC11, WGN+16, ZL+11].  Limit
[SN16b, Fra15, Fra16, LW16, LYC+13, OAN15a, SLT14, WTH+16].  Limitations
[LvG13a].  limiting [SLT+15].  Linear
[BG12, YN15, ZLY+16, ARLP13, CPV+12, EP12, FBY+17, FCE15, GZZ12, JzzM14, JMS13, LP11b, MA17, MSAK12, NYH+17, PH17, RS17a, RL+11, RR11, SS16a, Tak14, VBDS+11, WL10, YDX16].  linear-combination-based
[Tak14].  Linear-scaling
[BG12, YN15, NYH+17, RR11].  Linearity [IKN13].  linearized
[Fra15, Fra16].  Ling
[Ano12a].  Ling-Yun [Ano12a].  link
[HH15].  linkage
[HH11, OZS+13].  linked
[FO11, dACP12].  linked-cell [FO11].  linked-lists
[dACP12].  linker
[NPG17].  lipid
[BPPS17, MOS12, PGCT+12, ST11, WHAS+10, WHAS+16].  lipids
[HM16, ML14]. lipopolysaccharide [DLSA14].  lipopolysaccharides
[HBJ+17]. Liquid

methanol

methionine

Method

method

Methodological

methodologies

methodology

methods

methyl

methyl-methyl

methylacetamide

methylacetylene

Methylation

methylbenzyl

methylcobalamin

methylformamides

methyllysine

methyltransferase

Methyluracil

MetREx

metric

metrics

Mg

Mg-porphyrin-based

MHC

MIA-QSAR

micelles
Michael [NDG14]. microbes [RSLS13]. microclusters [NC12].
microelectrostatic [SMP17b]. microhydrated [SM17, ZYR +15].
microhydration [OSS10, SBD +17]. microiteration [SMM17].
WNM17, WRHF10, WKC11, WCAH10, XZ11, XTY+14. 

**model** [XP13, YOMT14, YB13, YSZ12, ZSTII14, ZKH+10, ZM10, dSddAR10, MJBM12].

**model-tuned** [HZS17]. 

**modeled** [MPA12]. 

**modeler** [KLJ+17]. 

**Modeling** [CB11a, DLSA14, FTW12, GMG+10, GBS+17, HPL13, JW16, Mat14, NS10, NDLW13, PLP+16, SK11, Tia12, Vyb15, AKMT11, Aou16, BEM14, BPC13, Bow16, BS10c, ČMD13, CLA16, CZNA11, DWR17, DSX+11, DLMH12, EBPK17a, FXC+13, GH10, GP12, GMZ12, GR10b, GWZX12, HLvdV13, HBJ+17, JC16, JCL+17, KSD+12, LABSG17, LLH14, LZGS11, LT13, LN15, MBA11, MJLV14b, MA17, MBA14, MPBJ11, NSO+14, NW17, PHC13, PSS14, PVT16, RJS17, SN16a, TTR+12, VKNT15, VAA14, VCM15, WXL17, WPM+15, WLO+12, XDL+10, XLY12, YJ11, ZX11, DHE12]. 

**modelling** [DBM+15].

**models** [BEM14, BLKP12, BPB11, CD11, Cor17, CBG16, CK17, DDP16, DSM+11, DLMH12, EBPK17a, FXC+13, GH10, GP12, GMZ12, GR10b, GWZX12, HLvdV13, HBJ+17, JC16, JCL+17, KSD+12, LABSG17, LLH14, LZGS11, LT13, LN15, MBA11, MJLV14b, MA17, MBA14, MPBJ11, NSO+14, NW17, PHC13, PSS14, PVT16, RJS17, SN16a, TTR+12, VKNT15, VAA14, VCM15, WXL17, WPM+15, WLO+12, XDL+10, XLY12, YJ11, ZX11, DHE12].

**modern** [AB16a, AB16b, DH17, Fom11, LMR14, SDM+16].

**modes** [CBP+15, GMPB12, LLTC12, MS17, dSAdSL13].

**modification** [Ano12u, MIS+15].

**modified** [BD12, CH16, DPSL16, DJX+11b, GSD10, MRO17, Mit13, SMM15a, SMM15b, SMM+18, XYX17, XVA+16, ZZ12].

**Modifying** [CYG+15, LB10].

**modular** [HPT+16b, JP15, LWK+14, MBR+15, PSG+17].

**modulate** [WC13].

**modulation** [PE11, RS17a].

**modulator** [ILKR11].

**modulators** [SRA17].

**module** [PHH+12, VBV13b].

**MOFs** [LPK16].

**moieties** [SPL+18].

**MOLCAS** [ADF+10, VBV13b, AAC+16].

**Moldyn** [HPSK12].

**Molecular** [AASP18, BDTP11, CRZ+18, ČMD13, Cor17, DHG+11, DHH+11, DSX+11, Fon13, Ibr11, JA10, KUDG12, KB14a, LWZK13, LBDP12, MFEM16, PL14, Pla11, RKG11, RO14a, RRK14, SBT17, SFLG+17, SV11, VSD10, WC11, WWKS11, XFG+16, XLY12, Yan16, YJXZ13, ZWS+10, AALCM11, AG11, AST+16, AFFF13, AS15a, ASL+11, AS10, APK14, AGB13, AS15b, AGR11b, AJR16, AB16a, ASK18, ALH+10, BMR11, BAMR13, BEM14, BSL11, BF15, BBOB16, BJS12, BU14, BW15, BF17, BJF15, BMBJ11, BE16, BVC13, BEL+11, CP14, CMM18, CM13a, CDBM11, CD13, Car14, CTR13, CAF+13, CBO15, CJKT13, CGPP11, CS14, CXW14, CBTZ16, CH16, COH14, CVG14, CCW+10, CHK10, CB11b, CB11c, CM16, DMM17, DSD+11, DJX+11b, DJX+11a, DLZ15, DDM+15, DL16, EP10, EK15, EJ13, EPH+13, ENKK+17, EPD+11, FBEM11].

**molecular** [FSC+14, GBL+11, GDV17, Gar12, GJMPAM+14, GSHM10, GR11, GMZ12, GPM17, GMMH+16, GFGS18, GY10, GWZ15, GCW14, GGM+12, GBW+14, GEP+14, GPdC+16, GP11b, GR10b, GPK12, EPH+15, HS17b, HB14, HS12, HCD+10, HDM+15, HPSK12, HH16b, HWLW11, HJ10, HXM+16, HHWL17,}
naphthol [CYY\textsuperscript{+17}, GZL\textsuperscript{+12}]. native [DJ13, HYL\textsuperscript{+11}, UCFR16, YL13].
native-like [UCFR16]. Natural [LCPS13, MBFP15, Wei12a, Wei12b, AO10, GMZ12, NC14, Sch12, GLW13a, GLW13b]. naturally [XVA\textsuperscript{+16}]. Nature [ABDGN12, MJM\textsuperscript{+15}, GPK\textsuperscript{+16}, HBR17, Kri10, LZJ\textsuperscript{+11}, LYL16, LdSR\textsuperscript{+16}, MLGB16, PKK17, RKM14, YK13, YJ17, ZRCC12]. navigation [SLG15].
NBe [UT14]. NBO [GLW13a, GLW13b, WvRSM14]. NBS [YZ17]. NCCH [MLGB16]. NCN [REV\textsuperscript{+17}, VVJ15]. NCX [LZL\textsuperscript{+15b}, LZL\textsuperscript{+15b}]. NCY [LZL\textsuperscript{+15b}]. near [DJ13, SISK10, Yan11]. near-native [DJ13]. near-solute [Yan11].
native-like [UCFR16]. Nature [ABDGN12, MJM\textsuperscript{+15}, GPK\textsuperscript{+16}, HBR17, Kri10, LZJ\textsuperscript{+11}, LYL16, LdSRR\textsuperscript{+16}, MLGB16, PKK17, RKM14, YK13, YJ17, ZRCC12].
navigation [SLG15].
NBo [GLW13a, GLW13b, WvRSM14]. NBS [YZ17]. NCCH [MLGB16]. NCN [REV\textsuperscript{+17}, VVJ15]. NCX [LZL\textsuperscript{+15b}, LZL\textsuperscript{+15b}]. NCY [LZL\textsuperscript{+15b}]. near [DJ13, SISK10, Yan11]. near-native [DJ13]. near-solute [Yan11].
native-like [UCFR16]. Nature [ABDGN12, MJM\textsuperscript{+15}, GPK\textsuperscript{+16}, HBR17, Kri10, LZJ\textsuperscript{+11}, LYL16, LdSRR\textsuperscript{+16}, MLGB16, PKK17, RKM14, YK13, YJ17, ZRCC12].
navigation [SLG15].
[CM16]. nitrolitro- [CM16]. nitrolitriacetic [CM16]. nitro
nitroaniline [ZTH+15]. nitroaromatic [PSC11, TD10]. nitrobenzenes
[ZGS+10]. nitrocompounds [SIG+15, SGH+16]. nitrodibenzofuran
[DPB+12]. nitroethane [YWL+15]. Nitrogen
[LLC17, BEPM14, KV14, ZZWX11, ZYL+12]. nitrogen-atom [KV14].
Nitrogen-doped [LLC17]. nitrogen-rich [ZZWX11, ZYL+12].
nitrogen-substituted [BEPM14]. nitroimine [ZYL+10].
nitromethane [MCUJ15]. nitrosamine [dALdS+15]. nitroso [TDP+12].
nitrosodimethane [TDP+12]. NMR
[Ben17, CHP11, EOA+11, HJ13, HBI17, HM13, KASH14, LK11, OPR16,
PTK11, PGdO+16, PC14, Pie14, RK15, SEF+16, SKMS13, WL14, YS13].
NNO [WGL+11]. NO
[MCUJ15, Ts17, ZZ10, WYGW12, BS16a, FYQ11, YSHG17]. noble
[ARLP13, JKS+16, PGS+15, PMG+16]. NOCV [CSM16, DBGO+17]. node
[KK17a]. nodes [KPF+15]. NOEs [LK11]. Non [KB11c, LCH10, CSHK15,
GMZ12, HOK17, MR17, NHI16, PHC13, RS13, YWJ+16]. Non-Boltzmann
[KB11c]. Non-Born [LCH10]. non-covalent [MR17, RS13].
non-electrostatic [HOK17]. non-equilibrium [NHI16]. non-heme
[PHC13]. non-hybrid [CSH15]. non-natural [GMZ12]. non-uniform
[YWJ+16]. nonadditive [RTS+13]. Nonadiabatic
[HZ11, JBSQ11, SRSLO15]. nonadiabaticity [Wu10]. nonbonded
Noncovalent
[dRCFGRB18, RRH12, SM16a, SBW12, TGR+16, VT14, WGD+16, YW13].
noncyclic [SM16a]. nonempirical [BK17b, WYT17]. nonequilibrium
[ASL+11, KHWB17]. Nonfitting [RZG+13]. nongeometric [KB11a].
noniterative [MS12]. nonlinear [ARLP13, KOP+14, LLD17, MLQ+12,
MIS+15, RLA+11, TFQ+10, Tia12, YCA10]. nonlinear-optical [KOP+14].
nonparametric [RB13a]. nonperiodic [MS15]. nonplanar [KG11].
nonpolar [LvG13b, MPSA17, PAT+10, WWW18]. nonpolarizable
[AOW11, WGD12, ZRL+15]. Nonrandom [NPP13]. nonredundant [HZ13].
nonspecific [CBP+15]. Nonstatistical [Yu12a]. nontemplate [OL13].
Nontotally [HOM+16]. nonuniform [BD12].
norbondenediene [Ant13, WJX+10]. normal
[GV+10, GMBP12, MS17, SBB10]. Notes [CD13]. Novel
[FCL+10, KKO+16, RPNP10, AIGP15, BEPM14, BPM15, DWF11, DMN14,
DFP+15, JYS+12, LLLC11, LLJ12, MPN13, PSDPE+10, RNP13, WKC11,
YJN+11, YHC11, YDGZ15, dCFLGL13]. novo
[AFBR17, BAMR13, LK11, MDT10]. Nuclear [ASK18, DKT13, ECZWD17,
KNP+12, CSEM+16, HHI16a, HII17, JKS+16, NASH15, RSG14, SS13b].
Nuclear-relaxed [ECZWD17]. nuclearity [BACSC11+10]. Nucleic
nucleobase \[ \text{ANH}^{+11} \] nucleobases \[ \text{WG}^{12} \] nucleophile \[ \text{ZYR}^{+15} \] nucleophilic \[ \text{MA}^{16}, \text{MLY}^{+13} \] nucleotide \[ \text{CBG}^{17}, \text{MJC}^{14}, \text{Ran}^{13} \] nucleotides \[ \text{DMN}^{14} \] Nucleus \[ \text{ZBB}^{16}, \text{FVB}^{10}, \text{TH}^{13} \] Nucleus-independent \[ \text{ZBB}^{16}, \text{FVB}^{10} \] nudged \[ \text{QB}^{10}, \text{QB}^{11}, \text{SH}^{11a} \] Number \[ \text{Ano}^{10b}, \text{ASMS}^{10}, \text{CLK}^{11}, \text{GPM}^{17}, \text{HMM}^{10}, \text{SL}^{10}, \text{SG}^{10b} \] numeric \[ \text{VI}^{17} \] Numerical \[ \text{WXL}^{17}, \text{CKKK}^{16}, \text{KEMP}^{17}, \text{KP}^{11}, \text{MBA}^{11}, \text{SLG}^{15}, \text{YS}^{12} \] numerically \[ \text{ZDZM}^{13} \] NUPACK \[ \text{ZSB}^{11} \] NWChem \[ \text{PGW}^{17} \] nylon \[ \text{BHNS}^{14} \] nylon-oligomer \[ \text{BHNS}^{14} \] O \[ \text{BCNH}^{+11}, \text{CX}^{50}^{10}, \text{DHE}^{+12}, \text{GBGR}^{16}, \text{HRL}^{11}, \text{JMV}^{14}, \text{LZ}^{10}, \text{LLL}^{11}, \text{LLB}^{+12}, \text{LSW}^{14}, \text{MG}^{11}, \text{PBE}^{16}, \text{RHT}^{+15}, \text{SPS}^{+12}, \text{SB}^{+17}, \text{V}^{14}, \text{WHL}^{+10}, \text{WRM}^{+12}, \text{XFX}^{+16}, \text{YW}^{12}, \text{YR}^{13}, \text{YOPB}^{16}, \text{ZRCC}^{12}, \text{Tsi}^{17}, \text{BCNH}^{+11}, \text{BW}^{10}, \text{CK}^{10}, \text{Chu}^{10}, \text{CRO}^{16}, \text{CPLL}^{11}, \text{DHE}^{+12}, \text{HZ}^{11}, \text{LZ}^{+15}, \text{LCW}^{10}, \text{MH}^{11}, \text{MS}^{15}, \text{PB}^{12}, \text{RNH}^{10}, \text{RAGL}^{11}, \text{SZ}^{17}, \text{SD}^{11}, \text{SSX}^{+14}, \text{YZ}^{15}, \text{ZRC}^{11}, \text{ZSWL}^{12} \] o-atom \[ \text{Tsi}^{17} \] O-loss \[ \text{MH}^{11} \] O-methyltransferase \[ \text{CPLL}^{11} \] OBC \[ \text{FCE}^{15} \] OBGMX \[ \text{Gar}^{12} \] Obituary \[ \text{Ano}^{15-60} \] object \[ \text{RLG}^{14}, \text{SK}^{15b} \] object-oriented \[ \text{SK}^{15b} \] objective \[ \text{PSG}^{+17} \] observables \[ \text{VZ}^{14} \] observed \[ \text{XML}^{+15} \] obtain \[ \text{GR}^{10a}, \text{GR}^{11}, \text{MA}^{16} \] obtained \[ \text{OSR}^{16}, \text{SISK}^{10}, \text{Tak}^{10} \] obtaining \[ \text{STM}^{17} \] occlusion \[ \text{BK}^{17a} \] occupancy \[ \text{MP}^{13} \] occupied \[ \text{HJJ}^{13}, \text{MRB}^{14} \] occupied-virtual \[ \text{MRB}^{14} \] occurring \[ \text{XVA}^{+16} \] OCF \[ \text{ZLL}^{12} \] octa \[ \text{ABDG}^{11}, \text{CC}^{18b} \] octa-1 \[ \text{ABDG}^{11} \] Octene \[ \text{MJLV}^{14a} \] OCXR \[ \text{FCOG}^{12} \] offsets \[ \text{KRSC}^{12} \] OFLOOD \[ \text{HNS}^{16}, \text{HNTS}^{15} \] OH \[ \text{CX}^{14}, \text{Chu}^{10}, \text{GTK}^{10}, \text{HZ}^{11}, \text{LLS}^{14}, \text{AR}^{10}, \text{CK}^{10}, \text{GK}^{10}, \text{LJ}^{+11}, \text{LJ}^{+11}, \text{RAGL}^{11}, \text{TJS}^{+10}, \text{VDVR}^{14}, \text{WLH}^{12}, \text{Z}^{+10a} \] OH/OD \[ \text{Chu}^{10} \] \( \cdot \) \[ \text{MVKS}^{10} \] OHHGe \[ \text{WHX}^{+10} \] oils \[ \text{SST}^{14} \] Ole \[ \text{Spr}^{10} \] olefin \[ \text{MJLV}^{14b}, \text{RS}^{17b} \] olfactory \[ \text{DR}^{14} \] oligo \[ \text{KSW}^{16}, \text{TZ}^{12} \] oligo-acene \[ \text{HZSS}^{17} \] oligomer \[ \text{BHNS}^{14} \] oligomerization \[ \text{ZQ}^{14} \] oligomers \[ \text{DP}^{15}, \text{PH}^{10b}, \text{ZSLL}^{17}, \text{TYW}^{+16} \] oligopeptides \[ \text{RS}^{16} \] On-the-Fly \[ \text{PAK}^{15}, \text{MIOM}^{13}, \text{PL}^{14} \] On-the-path \[ \text{CY}^{9}, \text{CY}^{13} \] One \[ \text{MBFP}^{15}, \text{COCOH}^{14}, \text{GAMAC}^{+14}, \text{HRID}^{16}, \text{KPL}^{13}, \text{L}^{10}, \text{L}^{11}, \text{L}^{13b}, \text{LvG}^{13a}, \text{PSC}^{11}, \text{RRK}^{16}, \text{SM}^{16a}, \text{SJ}^{11}, \text{SGH}^{13}, \text{WM}^{+10}, \text{ZZW}^{12}, \text{ZGS}^{+10} \] one- \[ \text{SJC}^{11} \] one-bit-per-sample \[ \text{HRID}^{16} \] one-bond \[ \text{RRK}^{16} \] One-electron \[ \text{MBFP}^{15}, \text{PSC}^{11}, \text{SGH}^{13}, \text{ZGS}^{+10} \] one-step \[ \text{LvG}^{10}, \text{L}^{11}, \text{LvG}^{13b}, \text{LvG}^{13a} \] ones \[ \text{YZ}^{15} \] ONETEP \[ \text{LCPS}^{13}, \text{WS}^{13} \] ONIOM \[ \text{AALCM}^{11}, \text{Gil}^{11}, \text{GWZ}^{12}, \text{Lun}^{12}, \text{Mor}^{15}, \text{RJW}^{12}, \text{TS}^{10a} \] ONIOM-ccCA \[ \text{RJWW}^{12} \] online \[ \text{Ano}^{12u}, \text{BJP}^{15} \] only \[ \text{LT}^{13} \] ONO \[ \text{WGL}^{+11} \] onto \[ \text{LL}^{13a} \] ontology \[ \text{CQFC}^{10} \] OOH \[ \text{LJG}^{+11} \] OP \[ \text{CSKH}^{16} \] Open
[HLS+13, Aki16, APK14, BG13, FBY+17, HPT17, ISO+13, KSD+12, NS17, PHT17, RJR14, SRR16, SMRM+17, XTG+11, Yap11, Yes12, CZH12].

open-ended [RJR14]. open-shell [BG13, ISO+13]. Open-source [HLS+13, Aki16, APK14, FBY+17, HPT17, KSD+12, PHT17, Yes12].


opsin [RLG11]. Optical [WGLG+16, ARLP13, BLL13, BLS10, GTT10, HB15, HRJ+14, HRJ+15, JRSHP14, KRT10, KOP14, LLBO12, LLD17, MLQ+12, MIS+15, MGS+16, MCK17a, TFQ+10, TFQ+11, TS15b, YB13, YCGA10].

optics [Tia12]. Optimal [WGLG+16, ARLP13, BLL13, BLS10, GTT10, HB15, HRJ+14, HRJ+15, JRSHP14, KRT10, KOP14, LLBO12, LLD17, MLQ+12, MIS+15, MGS+16, MCK17a, TFQ+10, TFQ+11, TS15b, YB13, YCGA10].


oral [LWL+11]. orbit [AMQ+14, FAA15, FD16, GP11a, JKS+16, MG11, PS17, YB11]. Orbital [WM12, ASL+11, BVC13, CIKT13, CPN+17, CGPP11, DFH+11, FE14, GWF11, GLW13a, GLW13b, IIF+10, IKN13, KTN10, LCPS13, LFN+10, LTP11, MFR+17, MGS+16, NF17, OHNK11, OOT15, OOK11, PRY1+17, PH15, RKGN10, SGPJS+17, Sch12, SMW09, SB14, SB15, TKN10, TS14, TSN16, US11, UM13, Wei12a, Wei12b, WCW15, WM17, ZA15, vLBBR12].


pairwise-additive [VMPS17].
palladium [WCWW11, YHG+11, dCDP15].
palladium-catalyzed [dCDP15].
paper [GPJSM12, Hl12, JW12, WM12, HP10a].
para [KYCL11].
para-substituted [KYCL11].
paracyclophane-bridged [KGR+16].
Paradoxical [UT14].
Parallel [BTB+11, KDB13, NN18, UIW+10, WWKS16, BW11a, BTT10, CEBO15,
CSSB11, GJMPAm+14, GRARO+14, HP10a, HS17b, HPSK12, KS13a,
KNHN16, KN17, KZZ+16, KJM+17, KDT+12, LL10a, LPLA13, MBR+15,
MCRL17, MYT+14, MJM+15, NNK+16, OPB+12, RFN15, SHMO11,
TCX+13, TJB12, WHK+12, Ys15, ZWL13, ZSS+13, CJL+13, KDT+12,
LMR14].
parallel-generalized [LL10a].
Parallel-ProBiS [KDT+12].
Parallelization [AB16b, VDL+13, BWMSM10, IUK+11, JMS14, KS15, KNN11, LLZa12,
RŠRR15, vW11, ZDKM12].
parallelize [vW11].
parallelized [DBDP16].
parallelizing [BMBJ11].
Parameterization [HK18, HJLV16, ILK11, IHJ+13, MPA17, PRRT+10, TCC+13, BAS14,
CCLP12, DLMH12, KYB13, LTP11, MSS+13, VLB+10, VBD11].
parameterizations [SH15].
parameters [OZS+13].
Part [HRJ+15, CDBM11, CD13, HRJ+14, Fer13b, SK13].
Partial [HTS17, JMILL13, SMP17b, WOH16, GVP+10, MPBJ11, PL14].
parsimony [UT14].
particle [AG11, BK13, Cas13, NO16, PH17, ZDKM12].
particle-field [ZDKM12].
particle-mesh [AG11].
partition [HGCCGR+16, JIS13, LRR13, WG12, WDHZ13, YAS13].
partitioning [DK11, EV14, FCOGM12, LZZ+17, REL17, SS13a, TMJ15, VGV+11].
partner [dVZ17].
passing [CSSB11, ZWL13].
Past [GS16, MFM16, XFG+16].
patches [OME16, YSSB12].
Path [MA17, VKAM12, CY09, HX+16, Ish10, JZ17, SRSLO15, SA13, SS13b,
SMML17, WXY+14, ZT14, CY13].
path-based [ZT14].
Path-integrals [VKAM12, WXY+14].
path-search [Ish10].
PathOpt [GPE13].
Paths [SH11a, AMGB10, Ant13, CX10, NMLD13, RVP+11].
pathway [BHR12, HOM+16, LKL10, SJ14, TDP+12, XLYZ10].
pathways [CM13a, EFB16, GS11, HNTS15, KGR+16, MTM14, QSW+10, QB16,
RCM+13a, RML+15, SJ11, SH18, Tsi17, WSH10, Yn16, BHB12].
pattern [CX10, WGL12].
Patterns [FZL+15, RS14].
Pauli [Ano15-60, Ano16-56].
Pauli [JH+13].
PAW [LGKS17, MDTD13].
PAW-based [LGKS17].
Pb [MCK17b, PMG+16, vSGP10, FBY+17, OBW12, vSGP10].
PB-AM
[FBY+17]. PBE [DOM+11, PTK11, LK16a, SGPJS+17, TG12a].
SV15, SEM12, TYZ\(^{16}\), XHLH16, YZ15a, dCLFGL13). peptide-backbone [HLH\(^{12}\)]. peptide-design [XHLH16]. peptides [BLKP12, BPC13, CCOH14, CZNA11, GFG11, HLH\(^{12}\), HHWL17, IO13b, JCX10, KB10, LvG13c, MZZ11, OLY17, WNM17, XHLH16, XWSW13, ZKH\(^{10}\)]. peptoid [MMZW14]. perception [AJR16, HYYZ13]. Performance [Abr11, BZB\(^{13}\), CSKH16, CKKK16, DOM\(^{15}\), HSB\(^{11}\), JCP14, LK16a, RKB\(^{14}\), SGWA17, ABM\(^{15}\), BLKP12, BPC13, CCOH14, CZNA11, GFG11, HLH\(^{12}\), HHWL17, IO13b, JCX10, KB10, LvG13c, MZZ11, OLY17, WNM17, XHLH16, XWSW13, ZKH\(^{10}\)]. peptide-design [XHLH16]. peptides [BLKP12, BPC13, CCOH14, CZNA11, GFG11, HLH\(^{12}\), HHWL17, IO13b, JCX10, KB10, LvG13c, MZZ11, OLY17, WNM17, XHLH16, XWSW13, ZKH\(^{10}\)]. pericyclic [HPT16a, KG15]. Periodic [Sce07, Sch10, AAC\(^{16}\), CMM18, CEBO15, FCD10, Gar12, HSH15, HBI\(^{17}\), ITIN15, KB14a, LBGS16, Man13, MGS\(^{16}\), NN18, NO16, NTNY15, RJPB12, SN16a, Sie15, TLdG12, Tak14, VBV13a, VBV13, VECT12, VI17]. Perlin [HLBLCCG15]. permeation [DMN15]. permutation [IO13b]. pernitrides [WD10]. perovskite [LLB\(^{12}\), LLL\(^{12}\), VVY17]. peroxide [KNP\(^{12}\), MK13b, SZ17]. peroxy [RHPWS13, RHT\(^{15}\), ZRCC12]. peroxy/superoxo [ZRCC12]. peroxo/persulphates [BLG11]. persistence [XW15]. Persistent [XFTW15]. perspective [ABDGN12, Dil15, Hsu14, JCGVPT17, JM\(^{+}\), LGOM\(^{+}\), MP17a, Niz13, PZM15, XLY12]. perspectives [DR14, Wei12a]. perturbation [CCM15, CF14, DCHL12, FRSA14, FSSW17, FE14, GR15, GCCM15, HI13, HRJ\(^{14}\), HRJ\(^{15}\), HYUS11, JRSHP14, KKKN11, KN17, KM13, LCL\(^{10}\), LLvG10, LLl11, LvG13b, LvG13a, MCC11, RLDJ17, RAR\(^{11}\), RHPWS13, SSSI15, TAG16, VDL\(^{+}\), WHAS\(^{+}\), YKH15, ZZ14, WHAS\(^{+}\)]. perturbation-selection [FE14]. perturbations [GMSdG15, OSR16, Tak10, WWCL15]. Perturbative [SSWX14]. perylene [BSL\(^{16}\), SLP\(^{+}\)]. perylene-based [SLP\(^{+}\)]. perylenediimides [QCR12]. pesticide [BBH\(^{17}\)]. peta [KNHN16]. peta-scale [KNHN16]. pecascale [SOCD13, ZWL13]. PH [LZL\(^{15}\), dSDAR10, LZL\(^{15}\), AB16a, CS14, CAD16, HS14b, MBA14, PZA15, PS13, SY16a, SOvG12, Vor12]. pH-dependent [SY16a]. pH-responsive [MBA14]. Phage [MP17b]. Phage-like [MP17b]. PHAISTOS [BFH\(^{13}\)]. pharmacokinetics [VBDS\(^{+}\)]. Pharmacophore [HRK\(^{+}\), HKRS11, HS11, TDO10, AKMT11]. Phase [ATM18, ZWMW10, ABD\(^{12}\), BE12, BG17, DLSD13, DLW12, EMD17, GYX\(^{+}\), Hsu14, KD10, LJJW11a, LPLB16, LGKS17, MFM\(^{+}\), NIIT15, PSC11, RWR\(^{+}\), RSLML12, RJS17, SJZ\(^{+}\), VKAM12, VED10, YHG\(^{+}\), YSG12, ZSZ\(^{+}\), ZWW10, ZYR\(^{+}\), ZLH14, dSDS12a, dSDS12b, ABD\(^{+}\)]. phase-change [EDEM17]. phases [EB12, LPAS11]. Phen [FD16]. phenol [AAMD\(^{+}\), AK10, PPH\(^{+}\), WHX\(^{+}\), YKH\(^{+}\), AK10]. phenol-imidazole-base [YKH\(^{+}\)]. phenol-triethylgermanium [WHX\(^{+}\)]. phenolates [SKGB13]. phenols [SK12]. phenomena [JBSQG11, WDP\(^{+}\)]. phenoxy [LY11]. phenoxy/phenol [LY11].
[SBW12]. PMF [ZLX +13]. PMMA [NNS15]. pmx [GMSdG15]. nicogen
[LDG +15]. pockets [MK11, TNSS17]. Point
[Lar11, AS15b, AGM +13, BHR15, BEL +11, BTB +11, EPD +10, LPS12,
LSW14, OHPR17, SN15, Tac17, TBSM12, Wei12b, YHW17]. points
[HDL +17, HEMCZE +14]. Poisson
[BCCO10, BD12, CLA16, FBY +17, FHMB15, FCE15, Fra15, Fra16,
GRARO +14, NWW17, SK15a, WL10, XYX17, YOMT14]. polar
[BK17a, CVG14, GMG +10, LvG13b, PAT +10, WWWW18]. polar-nonpolar
[BWWW18]. polarizabilities
[BLG +13, BZB +13, KR12, KNP +12, LIRL +16, MLC13, RLA +11, SS16b].
polarizability
[CPK12, EPD +11, HBKL10, KSK11, NYN17, OVPK15, PC14, YB13].
polarizability/reaction [KSK11]. Polarizable
[GEP +14, LPS +13, NS11, SAvG15, ZM10, BSL +16, Cam15, CCB15,
CGPP11, DGPM14, DGB +13, DDM +15, ENKK +17, ESM +12, FP17a,
GRS15, GPDc +16, HOK17, HZSS17, HCP15, ISO +13, KFY +13, KR12,
KWL +16, LRvdSM15, LFN +10, LHHW14, LDG +15, MBC11, MBC13,
MBE16, NLP +16, PMC +17, PZCL16, Ric16, SM14b, SK17, SbvG14,
VVLG17, WRHF10, WLO +17, XZ11, XP13, ZRL +15, ZP13].
Polarization
[Mit13, CD11, JZ12, LCW12, MLZZ12, POB13, RF15, TNG +10, WWD14,
YD17, ZJZM13, ZBG11, ZBP11]. polarizable [SS16b]. Polarized
[BS10a, BLG +13, DLZ15, JZZM14, NHF +10, SFM14, YJXZ13]. pole
[NYN17]. pole-search [NYN17]. pollutants [GCC14, SIG +11, TTR +12].
pollution [LZ14]. poly [CH10, PRRT +10]. polyacenes [KAR12, RS17a].
polyamidoamine [CAD16]. polyatomic [OT12]. polybrominated
[GKR13, Ray13, RKG11]. polycyclic [CB11d, FVB10, Kar17, PL18].
polyelectrolyte [DLP11, NNP13]. polyelectrolytes [NSP15].
polyethylenimine [BF17]. polylglycine [CCOH14]. Polyglutamine [PL18].
polyglurononate [Pla11]. polyhedra [CD16]. polyhedral [CL16]. Polymer
[HP10b, PH10a, MZZ11, SCMA +17, YCGA10]. polymer-growth [MZZ11].
polymerase [SBT17]. polymers [CRC13, GREA11, SA11]. polymorphic
[SLY +10, XWSW13]. polymorphisms [LXL +11]. polymorphs
[RRC +15, WRM +12]. polynomial [SY11]. polynuclear [CAT +13].
polynuclear metalates [CB11a, CB11b, CB11c, GLZ17, RDF +11]. Polypeptide
[AD10, IUK +11]. polyphenacenes [QZ10a]. Polyphilic
[vRWGS17]. polysaccharide [KSW16]. polyspherical [PH10a]. polyuronate [PD12].
poor [HDDH12]. populated [CBP +15]. population [LTA +11].
population-based [LTA +11]. Populational [DK11]. populations
[BVC13, KV13, OGL10, VZ14, WES13]. pore [KJ10, SFBT17, WNM17].
pores [DMN15, Fom13, HPL13, LJR +12]. porous [LZ14, PLZ17, SYZ +17].
porphyrin [BEL +11, EH13, INT18, KCK +15, PLZ17, VBMA13].
porphyrins [MLQ +12, TSNC +17]. portable [KS13a]. Porting [WS13].
pose [Vor10]. poses [HWLW11]. position [LHO17, VDVR14, BEEL14].
positive [SRA17]. positronation [BL12]. Possible

FCW+14, HRHI17, LLL+12, MO17, NFPD13, SMM+18, WDLG12].
pressures [RHNN10]. primary [ALK+15, GAI13, VVLG17, KTNN10].
[PSP15], principle [CCJC10, DBM+15, LLB+12, MCF10, Tak11, YPD13].
Principles [HFSO12, BE12, BE14, BPE16, EMD17, EB12, EBK13,
EBPK17a, GD10, HYL+11, Ibr17, JCG+11, LLLM11, LCWW10, NNS15,
PLZ17, RZG+13, SFA17, TZ11, WYL+15, WD10, YR13, wZbZ11, Zha12b,
Zha12a, ZWMW10, ZZ12, vADC+14]. principles-based [Zha12b, Zha12a].
prismane [DM15, VIT+15]. Pro [RB12]. Pro-Tide [RB12]. probe [RN17].
ProBiS [KDT+12].
problem [BB11a, GA14, KV13]. problems [HLX17, PWN+16].
procedure
[AD10, BK5+11, BY11, CJSZ10, HKR+14, MG14, MS12, SA13, dSAdSL13].
procedures [AC11b, CKH17, KSM16, PW12]. process
[ABDG112, BM12, DPAB16, HBL12, NIIT15, ZZ10]. processes [BPBL12,
FBEM11, HTS17, JM11, KV15b, LPLB16, PAK17, PTB+15, REL17].
processing [CKKK16, EP10, GBL+11, HASR+12, HEMCZ+14, WSGN11,
WS13, YWJ+16, YN15, ZKE+17]. processor [HCR12]. processors
[AB16a, AB16b, BDTP11, Fon11]. PROCOS [FHV+11]. produced
[LS11a, SIG+15]. Producing [RN17]. product [CC12b, ZQ14]. production
[GYX+10]. products [TR12]. profile [AK10, BS16a, KTT16, XML+15].
profiles [MIOM13, RBOH11, SISK10, Yu12b]. profiling [VMRS+17].
profit [KB11c]. Program
[FPV13, GH16b, SWA13, BBG+11, BBG+18, CBH14, CAT+13, FM10,
GLW13a, GLW13b, GBW+14, HS16a, HL14, JS17b, KWL+16, KK17b,
LHSH12, MHT+18, MSC+10, MsV12, Mez10, MSCP17, MB14, SFG+17,
SFR+11, SYN+12, TNYN16, TSC+13, VVV+15b, WCDM11, WHK+12, ZL11].
program/multiple [JS17b]. programming [LMR14]. programs
[LLC+10, PGL+15, PLAG11, vW11]. proguanil [APA+14]. Projected
[EF16]. projection [MDT13, HRCH16]. projector [BVH17]. prolapse
+[TH13]. proline [AS11, HJLV16, OOK11]. proline-catalyzed [HJLV16].
proline-recognition [OO11]. promelas] [TTL+12]. promising
[KSSH13, ZSL17]. promolecular [REV+17]. promoted [LPLB16]. Proof
[FVB10]. propagator [WWD14, YD17]. propane [WKC11]. propane-
[HSL+11, QSW+10, dSDdAR10]. Properties
[SFCCK+14, TY10, ARAG17, ASS10, ARLP13, ALH+10, BCSCJ+13, BE12,
BPE16, BLFZ13, BS10a, BACSCJ+10, BC13, CBH14, CWT+12, CWHH11,
CBTZ16, CH10, CCYL11, CXS10, CLC11, DDP16, DOM+11, DBM+15,
DPNM11, DJX+11b, DJX+11a, DP15, DLW12, DQ16, EBPK17b, FB10,
GBL+11, GTT10, GIK10, GWJJ12, GBGR16, EPH+15, HZY+10, HRR+17,
HLH+12, HZZS17, HLWD15, Ibr17, JBSQG11, JH+13, KP11, KDB13,
KZK+12, uLHY11, LHL+10, LHSH12, LLLM11, LZ1+11, LLD17, LBT11,
LBT12, LXX+10, LW1G12, MC10, MCF10, MJLY14b, Mat10, Mat14,

R [LdSRR16, NDG14, Sch10, LdSRR16]. R-C [LdSRR16]. R-Group
[ACS12, TSN16, BPC13, DXL+10, Gav12, RCM+13b, TTB+11, VÅA14].
relationships [CD13, Sti15, Wei12a, Wei12b].
relative [BLDK+13, CSS17, CM16, EOA+11, HH10, HH11, HDK+12, HLW+17,
Kar17, NHI16, PBLdS12, PPJ14, RLDJ17, RAR+11, RO14b, SOvG12,
ZRCC11, ZZ14, dALdS+15, dRBO13].
Relativistic
[ARAG17, BBI+11, GCCM15, RRK16, SNKS10, HKR+14, JKS+16, LHKS12,
LH14b, MCK17a, MCK17b, NASH15, OSHG17, PGdO+16, Pyy13, RK15,
TH13, VI17, ZXS+10].
relativity [JXSW15, SKMS13].
relaxation [KSH13].
Relaxed [YSRSS10, ECZWD17, KB14b].
release [KC13a, MBA14, PMT16, YDGZ15].
releasing [GMASBF16].
Relevance [TSNC+17].
relevant [ISP+10, KAR12, Mat10].
reliability [LLSW14].
Reliable [JZ17, LHG11, Kar17, NHN16, PBLdS12, PPJ14, RLDJ17, RAR+11,
RAR11, RO14b, SOvG12, ZRCC11, ZZ14, dALdS+15, dRBO13].
relocalisation [dCDP15].
Remarkable [BIL10].
REMD [PNW+16].
remote [BSDP16, RKDM14].
removal [LL13b, YS15].
renormalization [CAP17].
renormalized [ZMMM12].
Reoptimized [HLH+12, HH11].
reorganization [BE16, DAdGR15, RJS17].
Reparameterizations [DPSL16].
reparametrization [DH11, FCE15].
replacement [YHW17].
Replacing [ZSB+16].
Replica
[GS15, GS16, XFG+16, ZC14, CH16, CCOH14, IO13a, IO13b, KCK+17,
KT11, KTO13, LC17a, LMI+14, MS16, OGL10, OL13, OLY17, OZ14,
RFHG10, SBN13a, SB13b, TKI11, XFG+15].
replica-exchange [CCOH14, IO13a, KTO11, KTO13, LMI+14, OLY17, OZ14,
SB13a, SB13b].
replica-permutation [IO13b].
replicas [LL11].
Reply
[Can11, Cor17, GKR13, QB11, VVB13, WM12, LAT11].
representation [CXW14, CWOB10, FXC+13, HZY+10, KCPMG12, KDS17, LLC11,
ME10, YDL+10, YS10, YHH+13].
representations [OVPK15, dVZ17].
representative [KV12, KV13, VLGK+17].
representing [TY10].
repressor [OHNK11].
reproduced [Zha12b].
reproducibility [GKR13, Ray13, RK11].
reproducing [KTNN10, MAK+14].
reproduction [OPBR17].
repulsion [BBOB16, CGPP11, ENKK+17, HOK17, PS17, PC16].
repulsions [JJH+13].
repulsive [IO13a].
required [RAR+11, SG10b].
requirement [BF15].
requirements [TS15a].
requires [Bow16].
resampling [MMM+16].
rescaling [LL10a].
resoring [BMR11].
reservoirs [RFHG10].
residence [VBDS+11].
residual [LK11].
Residue
[LABSG17, BH15, BA11, GOM16, HIY15, NR11, SL10, SEF+16, WC14,
YHH+13].
Residue-centric [LABSG17].
residues
[FHK+12, KLS10, KML15, RK14, SK17, WXL+12, WC14].
resistivity [AB10].
resolution [BMFG16, BS10c, CM13b, DFP+15, Höfl14, JCC16, KN17,
NPG17, SM11, Vor10, WNM17, YN15].
resolution-of-identity [YN15].
Resolutions [LMR14].
resonance [EFS16, KN10+12, YB13].
resource [Gil11].
Response
[GPBS12, dSDS12b, BZH14, DHE+12, ESM+12, ITIN15, KSSH13,
KZK+12, LP11b, MRB14, RJR14, RCM+13b, SS16a, SDF+17, WGLG+16].
responses [GWX+12, MLQ+12].
responsive [MA14].
restrained

screenings [VKC10]. scripting [BK15]. Scrutinizing [SDM+16]..search [ACD+13b, MCAY15, Ran12, AIGP15, AGR11a, AC11b, DS15, GBSE11, GPE13, HRK+10, HKRS11, HS11, HEMCZE+14, Ish10, KM13, MS16, NYN17, Ng10, Ran13, TTRA+16, Vor10, XHLH16, XhD15, YZZ16, HTS15, ACD+13a]. searches [Pet11, RSL16]. searching [GK15b, HRK+10, HKRS11, HS11, LTA+11, ZYvIZ14]. Secondary [MCC11, TKN13, DCHL12, FSSW17, HIL13, ISO+13, KKN11, KN17, LCL+10, MLQ+12, yOTn16, SSB+16, TAG16, WYT17]. Second-order [MCC11, DCHL12, Hil13, KKNN11, KN17, LCL+10, MLQ+12, yOTn16, SSB+16, TAG16]. Secondary-order [MCC11, DCHL12, Hil13, KKNN11, KN17, LCL+10, MLQ+12, yOTn16, SSB+16, TAG16].


semiconductor [LCH+15, SFDE16]. semiconductors [BE16, NDLW13]. Semiempirical [SRL+15, GP11a, HGY15, KTN10, KB14b, LdS+10, MGWR12, SPH11, SDL14, TKN10, TG12a, UCFR16, WCWV15].

Sequence-based [TYZ+16, WXL+12]. sequence-reactivity [Sti15].
Sequence-specific [HYMZ16]. sequences [Ano12u, CCYL11, Fel10, HZY+10, LMZ+11b, LLLC11, LDH+14, OLA15, QLQ11, YDL+10].
Sequential [CBP14], SeR [LY10], serial [BR11a]. series
[AC11b, DDM+15, LZGS11, MCK17b, SRA17, SB10, TD10]. serious [BRKN12]. server [PZA15, XML+15, XYX17, dVAG16]. servers [UHH+11]. services [LP11a, UHH+11]. Set
[SN16b, BLL13, BLG10, BRLS08, BRLS12, CC11, HS16b, KNK+12, LS11a, LC+10, LYC+13, LWL+10, Mat10, OAN15a, PML+12, PGdO+16, PHK14, PD11, Pog10, PFVL14, RLD12, SPS+12, Sch13, SWM10, SG10a, SG13, VLGK+17, VVLG17, WX12, YOMT14, ZP+16, FL15]. Sets
[BWMSM10, SS+16, VV14]. Shao [Ano12u]. Shape [KC14, Zha11, GPS10, HCB11, Hsu14, MNNK10a, OAN15b, XTY+14, YLGX14]. Shape-based
[KC14]. shape-complementarity [GPS10]. shaped [LWZK13]. shapes
[CCOH14, Hug12, WS10]. sheets [PL18, WCAH10, YZW+17]. shell
[Ano15-58, BH14, BG13, GKS14, ISO+13, JCG+11, KSR17, MBA11, MA16, MS12, SRR16, TBSM12, WWD14]. shell-wise [KSR17]. shells
[GPK12, JXSW15]. Sheppard [QB11]. shielding
[GMZV14, HAI+16, PC14, VAMS14, YS13]. shieldings [JKS+16]. Shift
[BVHI17, Ben17, CHP11, DKE+17, EOA+11, FVB10, HJ13, JKS+16, KASH14, LK11, LZH+11, LS11b, MKH15, PTK11, Pie14, RK15, SEF+16, SK17, WL14]. Short
[DM15, Ibr17, LCCW10, MCK17b, TN12, UT15, AC11b, Cas14, DM15, HAI+16, JM11, LL13a, LDD17, SRS14, VIT+15, WKC11, YVEI+17, ZSL+11]. SIBFA
[DGPM14]. Si — [LYL16]. SiC [Kop16]. Side
[vRWS17, KLS10, KML10, LPS+13, LZGS11, LZZ14, LP11b, LvG13a, OZ14, QZM11, SA13, SISK10, SZBM13]. side-chain
[KLS10, KMLS10]. sidechains [GMZ12, PS13]. sigma [EPH+13]. sign
[DM15, VIT+15]. silica-bi [DM15, VIT+15]. silica [KKR+13, SIG+15].
silicalite \cite{CVG14}, siliceous \cite{Lar11, SN15}. Silico
\cite{VMRH17, AKMT11, AS11, DR14, EOO16, GS11, HS14b, LXL11, MPNS13, PVJ10, YLCX10, GMASBF16, CV12]. silicon
\cite{AC11b, BIL10, DM15, EFOD13, GSSM15, KOP14, Op16, KZK12, TN12, THP15, VT15, XhD15]. silicon-doped \cite{TN12}, silicon-germanium \cite{GSSM15}. silver \cite{YXZZ17}. silylene \cite{BIL10}.
Similarity \cite{HS12, LMZ11b, YDL10, CDM10, CDB10, CDBM11, CQFC10, GWT17, GK15b, HRK10, HKRS11, HS11, RMPAM15, YZZ16, ZYvIZ14]. Similarity/dissimilarity \cite{YDL10}.
SIMONA \cite{SWB12}. Simple \cite{Ano15-59, CNK97, GM17, MPSA17, AB16b, BS10b, BD12, CWZB10, TN12, THP15, VIT15, XhD15}.
simplify \cite{BLZ13}. SIMPRE \cite{BCSCJ13, BCJC14, KR14}. SIMPRE1.2 \cite{CSEMB16}.
Simulaid \cite{Mez10}. simulate \cite{SLX15}. Simulating \cite{BRE16, MFEM16, RKDM14, XFG16, Aki16, BTA13, BM12, BDTP11, BW15, BF17, JPG15, BMBJ11, BB11b, BB11c, BB11, CTR13, COOH14, CVG14, CLK11, DGH11, DNM14, DSD11, DHH11, DZT11, DSK17, DLZ15, DMD15, EK15, FTW12, GBL11, GR11, GMP17, GCW14, GP1b, Has14, HCD10, HFISON2, HPSK12, HDPM14, HMM10, HYUS11, HJ10, HHWL17, IPAA11, JIS13, JWO15, JMS14, KV13, KCK17, KCK15, KvdV14, KGKH12, KGHC15, KLO10, KB11a, KTO11, KSR16, KLS10, KMS10, KWL16, Kv15a, KPF15, LH11, LC17a, LRvSM15, LZ12, LPS13, LMI14, LZLM16, LAS14, MN15, MCRL17, MTvG12, MFEM15, MADWB11, MKM17, MB14, NST14, NFDP13, NKN16, NTNY15, Oht16, OCL11, OLY17, OZY1, OCW15, PGO15, PH17, PZCL16, PL14, PM13, PS13, PS10, PNG10, Rd14a, RLG14, RS11R15, SBV10]. simulations \cite{SS13b, SBT17, SISK10, SJ17, SMP17a, SYN12, SK13, SFLG17, SB15, SWB12, SDMS13, SV11, VSA11, VKTRJ15, VM11, WLIC12, WAM17, WH11, WWSK11, WLC12, WBF17, WG14, WC14, XFG15, XWSW13, YK011, YSG12, Yon16, YHVM12, ZZY16, ZDKM12]. simulator \cite{BSL11, KJM17, RLLHL12, TCX13}. simultaneous \cite{LL10b}. Single
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PG14, RLLHL12, RNSF$^{+16}$, Ras17, Řez16, RR14, RdA12, RSR$^{+12}$, RCM$^{+13b}$, SM14a, SFG$^{+17}$, SK15b, SWA13, SMRM$^{+17}$, She12, SC15, Sie15, SJ17, SWB$^{+12}$, SDMS13, TNYN16, TSC$^{+13}$, TTR$^{+12}$, TTL$^{+12}$, UU12, VMRSH$^{+17}$, VVV$^{+15b}$, VAR12, VBV13b, WdVN12, WDY13, WPM$^{+15}$, WF16, Wei12b, WKH$^{+12}$, WHJI13, WGI14, WCJ$^{+14}$, XML$^{+15}$, XYX17, YWJ$^{+16}$, YZZ16, Yes12, Yes15, YHH$^{+13}$, ZDKM12, ZLL$^{+13}$, dVAG16, CCC$^{+11}$, DBF14, MSvG12, MJG$^{+15}$, SBV10, SGM$^{+13}$, Yap11, ZCS$^{+15}$, She12]. softwares [All$^{[11]}$]. solar [ACS12, DGL$^{+13}$, JYS$^{+12}$, LZL$^{+15a}$, SLC$^{+17}$, TZ12, VAA14, YJN$^{+11}$]. Solid [RSK$^{+15}$, AS10, AS18, CL16, HLS12, HBI$^{+17}$, KLN12, POB13]. Solid-state [RSK$^{+15}$, HBI$^{+17}$, KLN12, POB13]. solids [BK11, HAI$^{+16}$, MTD13, MS15, dRL11, Pon11, SN16a]. solubility [KKO$^{+16}$]. solute [BRLS08, BRLS12, EOAI$^{+11}$, TKT11, YKO$^{+11}$, Yan11]. solutes [GC11, PAK15]. solution [AvKSP16, AK10, DR11, DBM$^{+17}$, DP15, EOAI$^{+11}$, GAI13, GAI14, HKD$^{+12}$, HAL14, HN$^{+17}$, KTN10, KVR10, LVG10, MM$^{+17}$, MF$^{+12}$, PMC$^{+17}$, PGW$^{+17}$, SJWE10, TKNN10, UCPR16, WHL$^{+10}$, WC13, XTG$^{+11}$, ZLL$^{+10}$, ZZ10, vADC$^{+14}$]. solutions [Ber17, CFC15, EK15, Kri10, OCW$^{+15}$, SM14a]. Solvation [RNSF$^{+16}$, ZBP11, CBG17, CBG16, FGM11, GMH$^{+16}$, GPK12, HRC13, JMLL13, JGS$^{+17}$, Jor17, KSK11, LP11b, MS13, MPSA17, MBE16, NW17, OW17, PL14, RK16a, RK16b, SM14a, SK12, SY11, SMM15a, SMM15b, SM$^{+18}$, TKYN17, TCC$^{+13}$, WXL17, WWW18, YOMT14, YAS13, Yan14, ZCS$^{+15}$]. solvation-free-energy [SMM15a, SMM15b]. solvational [FCL$^{+10}$]. Solvatochromic [MKH15]. Solvatochromism [TKYN17]. solve [PNW$^{+16}$]. Solvent [KC13b, AKK$^{+16}$, BEM14, BRLS08, BRLS12, CAD16, CBG16, EK15, FZ$^{+12}$, FD16, HLD$^{+17}$, Has14, HYUS11, KJDB12, KB11b, KCPMG12, LHL$^{+10}$, LC17b, LLL$^{+16}$, LWZ$^{+17}$, MBC11, MBC13, MS11, ML14, MCC2015, MNN10a, MNN10b, PDM10, PS13, RdA12, RR16, SLT14, SBV10, SK17, SLX$^{+15}$, SYH12, SCMA$^{+17}$, SKMS13, TYN15, WWS11, WXL$^{+12}$, WBF17, YOMT14, Yan14, YJJ1, BR17a]. solvent-dependent [HYUS11]. Solvent-driven [KC13b]. solvent-induced [AKK$^{+16}$]. Solvents [LHT15, ISO$^{+13}$, Ple14, Pog10, RK16a, RK16b]. solver [FY1$^{+17}$, FHMB15, Kan15, SHF11]. solvers [GRARO$^{+14}$, WL10, XYX17]. Solving [KV13, SG10a, BYE$^{+16}$, GA14, SK15a]. solvolysis [OSS10]. SOMA [BMFG16]. Some [RCM$^{+13b}$, CME11, CCL18, CCYL11, CXX10, MLVL14b, Byb16, ZPF14]. sometimes [VDRV14]. Song [JW12]. Soon [A016-75, A016-80, A016-81, A016-82, A016-83, A016-84, A016-85, A016-86, A016-87, A016-88, A016-76, A016-77, A016-78, A016-79]. soot [KAR12]. SOP [AKK$^{+16}$]. SOP-GPU [AKK$^{+16}$]. Sorafenib [GMASBF16]. Sorting [NMF$^{+14}$]. Source [TCB16, Aki16, APK14, BZH14, CD13, FY1$^{+17}$, HLS$^{+13}$, HPT17, KSD$^{+12}$, PHT17, SMRM$^{+17}$, XTG$^{+11}$, Yap11, Yes12]. sources [BK13]. Space [vRWGS17, ACD$^{+13a}$, ACD$^{+13b}$, AD10, Cas13, CH16, CXX10, DK11, GA14,
Standard
[DH17, BCJC14, MKO13, PNI13, REL14, SRR16, VVG13, WHK12].

standing [TS11]. staple [SV15]. Star [MA17]. State
[CCM15, GS16, Alg17, AR10, ASS10, BS15, BBI11, CSAO17, CH10, CV12, ESM12, FD14, GS15, GCCM15, GPE13, HLS12, HNF07, HNWF12, HH16a, HH17, HBI17, HZSS17, HBR17, JZ17, KLN12, Kop15a, Kop15b, KKL13, KCL14, LGL11, LvG13b, LL10c, LLBO12, LWGZ15, LN15, LGG11, LLF16, LXFC17, MTM14, MPSG11, MCC11, MC12, MCLD10, NYN17, NMLD13, OBW12, OZLSB12, PBO13, PGW17, PH10b, QZ10c, RAGL11, RIJ11, RML15, RR14, SRR17, SSSM15, SGWA17, VZ14, VL17b, WHL10, WHX10, YWZ14, YD17, YYT12, YL13, Zim15]. state-selected [KCL14]. State-specific
[CCM15, GCCM15, LGL11, LXFC17, MCC11, MC12].

states
[AST16, ANH11, BSL16, DHO13, EFS16, EK17, EP15, FAA15, FD16, GO13, GA12, GTK10, HDHL15a, HDHL15b, HDHL15c, JCGVP17, KB14b, LLBO12, LW12, LWW12, LX11, LS11b, LYSS11, MS10, MN15, MH11, PBDW11, RHRCH16, SRF17, SOYC12, SB15, SZSS16, TN10, Tia12, TSN17, VVV15a, XWSW13, YZGS14b, YK13, YLZ10, YB11, ZXS10, ZBB16, dLC17]. Static
[KBC12, BS10a, KZK12, Lu11, PC14, PNW16, PM13, WYT17]. Statics

Statistical
[FBEM11, KERY16, MJC14, NFG13, SJ17]. step
[AYYO17, DS12b, DG14, GRCL12, JWO15, JS17b, KvdV14, LVG10, LGL11, LvG13b, LvG13a, LL10c, RLDJ17, RS12, SJC11, TCP14]. steps
[REH13, Zim13]. Stepwise
[DL11, GRCL12, ZL11]. stereochemical

Stereoselection
[BJSI12]. Steric
[RMGB11, MJLV14b, MP17a, YNH17]. sterically [MH17]. Stern [MBA11]. stereoelectronic [HLBLCC15].

Stevens
[BCJC14]. sticks [CVT11]. stilbene [BW11b]. Stochastic
[AFPI13, CGP12, AC12, KV12, KV13, MS16, NC12, PH17, RSL13, SW12, VBD11]. STOCK
[BJ15]. stoichiometric [VI17]. stoichiometry [FSD18]. Stone
[DUZ17, YZN13]. stool
[FPB12, FBJ14b, ZCK16]. storage
[BEM14, BEMP14, DL17, WK12].

Story
[Sce07, Sch10]. Strain
[DM15, FB12, FC16, FLM11, JWO15, PBE16, SHE12, SHL13, V15].

strand
[XLY12]. strategies
[AFBR17, BSDP16, cCVG14, DSX11, LTT16, RAO11, SCOJ13]. strategy
[CLX10, CZNA11, HJKJ13, KTN10, LLL10, PHC13, PH17, RVK13, TKNN10, WO15, XHL16, YDG15]. strength
strengthening [MS11, LYSS11]. strengths [CKL+11, MLC13]. streptavidin [MLZZ12, ZJZM13]. streptavidin-biotin [MLZZ12]. streptocyanines [WYT17]. stress [GMBX+16, HXM+16, JMX+16, NIIT15, NFI+16, XFX+16]. stretching [CK10, RS17b]. string [BMFG16, JZ17, Zim15]. stringent [DPOS16]. strong [Kan15, MLZZ12, SDF12, VVY17, Vik11, ZSLL17]. stronger [KSC16]. Structural [GLF16, GBL+11, GTT10, GAMAC+14, GWX+12, HS17a, I110, KKK+12, KSD+12, LBTV11, NC14, TS11, ZWW10, AIGP15, AD10, AKK+16, ALI+10, BBOB16, BPC13, CPV+12, CDS16, CYI+10, DWL11, DH11, GWT+17, HS17b, HVS16, KKPT11, KG11, KNE11a, KDT+12, LK13, LL13a, MCF10, PHC13, PGP15, PNG10, RRF11, RKB+14, RSL16, SFA17, SS13c, WC11, XMSZ16, YVEI+17, ZLW10, VPR10]. Structure [BJP15, CGBK13, DXL+10, GPK+16, GWJJ12, GBGR16, HLB15, LAHS16, MHRR11, NC12, NC13, PMG+16, Rab12, SGH+16, VDVR14, WZK+13, APFI13, AR15, AJR16, AC12, BPPS17, BFH+13, BDD13, CD13, CM13b, Clo15, DKE+17, DKT13, DDP16, DVVP14, DLW12, EH13, EWF+13, EFOD13, FZY+12, FSC+14, GLB16, GMSiG15, GRARO+14, GP12, GK10, GRD+10, GpIC+16, HASR+12, HNHR13, HS14a, HRB+17, HH15, HYM16, HZ13, HLWD15, Ha16, Ibr17, KTY+17, KSM17, KT10, KS12, KKL+13, KLS10, KMLS10, LLBO12, LFB14, LKL10, LZ13, MRI+14, LLY16, LPE+10, LGL11, LHG11, LWWG12, LLFI16, Mat10, MDT10, Mau14, MAP10, MV17, NGAS17, OCL11, OL13, OLA15, PSS14, PML+12, PN13, RLG14, RM+13b, RR11, SHMO11, SB10, SM11, SLP+12, SLL12, SRS14, SYN+12, SKGB13, TN12, TTB+11, TGI2b, UNT16, VV12, VH16]. structure [VBL17, VA14, VBMA13, VKC10, VI17, VLG1+17, WO15, WR+12, WSGN11, YW12, YZZ16, ZRCC11, ZHHX11, OSF12, SA10]. structure-activity [DXL+10]. Structure-based [CGBP13, DXL+10, DVVP14, GLB16, VKC10, YZZ16]. studied [Ish10, KRTB10, OLY17, RHPWS13, RI10, TS15b]. Studies [JW12, AALCM11, BLS10, BRGN12, BLG10, DMN15, BIL10, DIL10, GZZM16, GEP+14, JLS+10, KG15, KP11, LXFC17, LCWW10, LJL+11, LW13, RC+13b, SB10, SFA17, SLHW09, TDP+13, VSD10, WCAH10, YKH+10, YPC+10, YDL+10, YXXZ17, ZZL+12, ZZL+10a, ZYG+15, ZX11]. Study [JLH+14, VL17b, AARP17, AS11, AS15a, AMAA+11, ASMS10,
study [LZL+10, LCL+10, LZJ+11, LZHH11, LWL+11, Li+14a, Li+14b, LGW12, LT13, LJW+11b, LBT11, LBT12, LTP11, LYSS11, LHKS12, LH4b, LLSW14, LWXC16, LHT15, Lu+11, LGJ+11, LPMT17, MMS16, MC10, MG15, MCF10, MJLV14b, MAPB10, MFM+12, MH11, MWJ+11, MS11, MPNS13, MHR11, MBRC16, MO17, Mor+15, MIS+15, NHF+10, NGAS17, NASH15, NC12, NC13, NC14, NJX+10, NFT+16, OPR16, ORZ11, OSS10, OSHG17, OME16, OOK11, PVL+13, PGCT+12, PP10, PG12, PG5+15, PH12, PAK17, PPH+14, QYL10, QZJ0b, RS17a, RAGL11, RAR+11, Ray13, RS13, RS14, RVCF13, RSLML12, RKG11, RSKG14, SN16a, SSP+13, SGDT10, SJD14, SCM+15, SRF+17, SWM10, SBD+17, SNS16, SGS+16, SE14, SCMA+17, Su+10, SKY+11, STS+10, SKTT11, SZS16, STS15, SGHL13, SIG+15, TM16, TLA10, TSNC+17, TSR+16, TL16, VKNT16, VPR10, VAR12, Vik11, VL1GK+17].

study [VED10, WKC10a, WHL+10, WCWW11, WDL12, WLL12, WYL+15, WNM17, WHX+10, WD10, WMW+10, WQW10, WS11, WHD11, WCL+11, WYGW12, WDP+12, XDL+10, XZ11, XWW+11, YZS14a, YZWC11, YHG+11, YZN13, YR13, YJXZ13, YLZ+10, YKH5, YSRSS10, YCG10, YB11, YYT12, YZ15b, ZCK+16, ZWGO16, ZTH+15, ZPP+16, ZXS+10, ZZZ+10b, ZZZT12, ZYL12, ZLL12, ZSZ+14, ZDX11, ZYW+10b, ZYW+10a, ZBP11, ZZZ2, ZZZX11, dSDAR10, dSDS12a, dSDS12b, dSLBN17, dLAoS+15, vADC+14].


substituents [CBTZ16]. substituted

[AR11P, BEMP14, CCLCRO14, CZH12, DCHL12, KY11L, KV15b, LHZ16, LWL+11, LTP11, Lu+11, OS12, PRRT+10, QCR12, SSP+13, SK12, SKGB13, UT14, WGL12, YPC+10, ZZWT12]. substitution

sulfide [LAW+16, ZYG+14]. sulfides [OSF12]. sulfonyl [YHVM12].
sulfonyl-containing [YHVM12]. sulfoxide [GC11]. sulfur
[CTR13, HS14a, HS16b, Kop17b, OSF12, WGL12, YB11, ZM10].
sulfur-containing [YHVM12]. sulfuryl [YHVM12].
sulfoxide [GC11]. sulfur [CTR13, HS14a, HS16b, Kop17b, OSF12, WGL12, YB11, ZM10].
sulfurization [TR12]. sum
[SB13, SB15, Tak14, Tia12]. sum-over-states [SB13, Tia12]. sumanene
[CLFRO18, CBTZ16]. summation [GBFD12]. summations [SB13].
superalkali [LLD17]. superatom [LYL16]. supercharger [FRN15, RFN15].
supercomputers [KNHN16, KN17]. superlattices [KC13b].
supermolecule [XZ11]. superoxide [GEP+14]. superposition
[CDBM11, HS12, PD11, YLGX14]. superpositions [KB11b, LAT10, LAT11].
Supersecondary [ZHHX11]. supervised [DGPM14]. support [HJ13, RLL+10, TYZ+16]. supported [SN16a].
supramolecular [CSGOA17, HLB15, OAN15b]. Surface
[LK16a, SRS14, Ano15-58, BPM15, BH14, CM13a, CR14, Che17, DBM+15, DS12b, FZY+12, FMNC11, FVP14, GCWS15, GY10, HLvdV13, HWLW11, HYD10, JZ17, JCX10, KKR+13, KTSW11, Kop16, Kop17a, Kop17b, LLH14, LL13a, LYC+13, LWZ+17, MK13b, MAK+14, MB14, MOS12, NW17, OKIS17, OHPR17, PZA15, SRSLO15, SH14, SBC+11, SLG15, SLLL13, SIG+15, TSR+16, WXL+12, WXL17, WBF17, XFX+16, YPV13, Yan14, ZLT13, ZKE+17, MK11]. surface-enhanced [SLLL13]. surfaces
[AKN16, BHB+17, BS16b, CCJ+11, CSXZ17, CZNA11, GFG11, Hei10, HRL11, IN13, KLS10, KMLS10, LX11, LAW+16, MCC11, MSc+10, MCF10, NPP13, Pol13, RNNS+16, RRC+15, RBHO11, SRF+17, SFR+11, SC15, SFLG+17, TG12a, VT14, WKC+10b, YZ15a, YR13]. surfactant [WWKS11].
SurfKin [LLH14]. Surprisingly [KG15]. surrounding [BSL+16]. survey
[GRARO+14, SJD11]. Surveying [KB11b]. Sust [Ihl12]. Suwa [MO15].
SVM [XWW+11]. swarm [LZL+13]. SwissParam [ZCGM11]. switch
[LCB10, MJ+11, MB16]. switchable [MLQ+12]. switching
[AB16b, KOP+14, LCH10]. symmetric [HOM+16, KZK+12, LPS12].
symmetries [GR10b]. Symmetrization [MSK+10, MSK+12].
Symmetrizer [LPS12]. Symmetry
[CAA10, EP15, VV+15a, BV14, CWZB10, DZA11, Dry14, FF11, HB14, KTT16, KC13b, NDD+10, PZBA13, Sch13, VGLT16, YHK15].
symmetry-adapted [FF11, YHK15]. symmetry-invariant [CWZB10].
synchronicity [dSvdM+16]. synthase [AALCM11, SYH12, XLYZ10].
synthase-catalyzed [XLYZ10]. synthesis [ZZWT12]. synthetase [LBS10].
syringe [ZWS+10]. system [BEEL14, BT710, BCCO10, CS14, CIJZ10, GRS15, HSY+11, HDM+15, LL11, LLY16, LZY12b, MLZZ12, NTNY15, NS15, RHT+15, SZBM13, TL16, VBDS+11, WLF11]. Systematic
[GP11b, ML14, SA13, SCMA+17, UT15, VLGK+17, AIGP15, BEL+11, FM10, Ish12, LG11, Pet11, STS15, VVGL17, WG12, RFHG10]. Systems
[RMM16, AST+16, APK14, BV14, BVY+12, BK13, BBG+18, BG13, CSS17, CEBO15, CKL+11, CLK11, CAP17, EP12, GG10, Gar12, GP12, GBW+14,
GR10b, GWZX12, HS11, HCD+10, HvM16, ITIN15, JSXH16, JS17b, KV12, KGM12, LBGS16, LPCS13, LPLA13, MSC+10, MG14, MOS12, MS12, NYN17, NCV10, NFG+13, NO16, NKK+16, NS17, OPB+12, OC14, PAK17, PAT+10, PBBP11, PD12, RJPB12, RVCF13, SCOJ13, Sch12, Sca10, SH18, SWB+12, SG13, SMM17, TSN16, TCX+13, UT15, WCY+11, WWU12, WS11, YCK16, ZSB+11, ZT14, HvM17].

tetraamines \[SB10\]. tetracarboxylates \[CRC13\], tetracoordinate \[XhD15, ZYW+16, ZLY+16\]. tetraene \[ABDG12\]. tetramer \[ish10\]. tetraradical \[Cas14, YSSB12\]. tetraoxide \[JW12, SLHW09\]. tetraprotonated \[ZWY+10b\]. tetraradical \[Cas14, YSSB12\]. tetrasaccharide \[NPG17\]. tetrathiafulvalene \[MCF10\]. Tetrazine \[JW12, MCAG+16, SLHW09\]. Tetrazino \[JW12, SLHW09\]. Tetrazino-Tetrazine-Tetraoxide \[JW12, SLHW09\]. tetrel \[YKH15\]. tetroxide \[MCAG+16\]. text \[HKRS11, HS11\]. text-based \[HKRS11, HS11\].


Theoretical [AvKSP16, AMAA+11, BHB+17, BSDP16, CWT+12, DBM+17, DGL+13, FF11, GYX+10, GLZ+17, GLM+17, HDHL15c, JW12, KCB+12, KS13b, LCL+10, LLY+11, LLW+12, LZY+12a, LWG+12, LWXC16, LXFC17, LYG+11, MLQ+12, MSV+16, NFI+16, OAN15b, PKK+17, PM+13, PE11, RS+17b, SB10, SKY+11, STS+10, ZZS+16, SLC+17, SGHL13, TPL+10, WMW+11, WHDL+11, WCL+11, WS12, YJN+11, YPC+10, YHG+11, YCG+11, YTC+11, CB+16, DLT+17, DSM+11, GPM+17, HJ+13, JMML+13, JHMB+09, JHMB+11, KG+15, NKE+11a, KRSC+12, NYH+17, SBR+13, TAK+11, TY+10, TS+11, VJ+15, VYY+17, VYBL+17, XDL+10, ZWY+10a].

determine [CDB+10, KSH+13, YBH+11, CRZ+18, MCC+12, ZWL+10].

Theorem [CDB+10, KSH+13, YBH+11, CRZ+18, MCC+12, ZWL+10].

Theoretical [AvKSP16, AMAA+11, BHB+17, BSDP16, CWT+12, DBM+17, DGL+13, FF11, GYX+10, GLZ+17, GLM+17, HDHL15c, JW12, KCB+12, KS13b, LCL+10, LLY+11, LLW+12, LZY+12a, LWG+12, LWXC16, LXFC17, LYG+11, MLQ+12, MSV+16, NFI+16, OAN15b, PKK+17, PM+13, PE11, RS+17b, SB10, SKY+11, STS+10, ZZS+16, SLC+17, SGHL13, TPL+10, WMW+11, WHDL+11, WCL+11, WS12, YJN+11, YPC+10, YHG+11, YCG+11, YTC+11, CB+16, DLT+17, DSM+11, GPM+17, HJ+13, JMML+13, JHMB+09, JHMB+11, KG+15, NKE+11a, KRSC+12, NYH+17, SBR+13, TAK+11, TY+10, TS+11, VJ+15, VYY+17, VYBL+17, XDL+10, ZWY+10a].

determine [CDB+10, KSH+13, YBH+11, CRZ+18, MCC+12, ZWL+10].

Theorem [CDB+10, KSH+13, YBH+11, CRZ+18, MCC+12, ZWL+10].

Theoretical [AvKSP16, AMAA+11, BHB+17, BSDP16, CWT+12, DBM+17, DGL+13, FF11, GYX+10, GLZ+17, GLM+17, HDHL15c, JW12, KCB+12, KS13b, LCL+10, LLY+11, LLW+12, LZY+12a, LWG+12, LWXC16, LXFC17, LYG+11, MLQ+12, MSV+16, NFI+16, OAN15b, PKK+17, PM+13, PE11, RS+17b, SB10, SKY+11, STS+10, ZZS+16, SLC+17, SGHL13, TPL+10, WMW+11, WHDL+11, WCL+11, WS12, YJN+11, YPC+10, YHG+11, YCG+11, YTC+11, CB+16, DLT+17, DSM+11, GPM+17, HJ+13, JMML+13, JHMB+09, JHMB+11, KG+15, NKE+11a, KRSC+12, NYH+17, SBR+13, TAK+11, TY+10, TS+11, VJ+15, VYY+17, VYBL+17, XDL+10, ZWY+10a].
time-dependent [JYS+12], therapeutic [AFBR17], therapy [ZZ12], there [MLGB16]. Thermal [LL10c, ASL+11, BIL10, NGA17, OZLSBH12]. thermally [HIY15], thermocalc [HDH12]. Thermochemical [TFQ+11, KSM16, TN12, WD12]. thermochemistry [HDH12, Sán17, SB14]. Thermodynamic [EOO+16, PAT+10, BE12, BPE16, BB11b, BB11c, CBH14, CC18a, EBPK17b, HDL+17, Hug12, MMB+17, PGY15, PBE16, RNSF+16, RRF11, RKB+14, SS13c, SJC11, SJ16, WC11, dRBO13]. Thermodynamics [DS12a, RS12, BPE16, DMJ17, EHSPT16, HRC13, Kan15, WRM+12, ZYL+12].


Three-residue [NR11]. threshold [LCM16]. throughput [ESB13, JBAM11, PVJ10]. thymine [HvM12, LJW11a, SBD+17]. thymine/thymine [HvM12]. Ti [WWK316, YW12, BH15, SBD+16]. Tian [Ano12a]. Tide [RB12]. Tight [Lar12, GAI+17, HNW07, HNW12, JCP14, KZZ+16, MFR+17, NF17, NN18, NO16, NKK+16, Oht16, SPS+12]. Tight-binding [Lar12, HNW07, HNW12, JCP14, KZZ+16, MFR+17, NF17, NN18, NO16, NKK+16, Oht16, SPS+12]. Time [GTK10, PAK17, WHL+10, WHX+10, YLZ+10, ZDX11, AYY017, CHG+16, DGC14, Fom11, FSSW17, HCD+10, HNW07, HNW12, HG10, JWO15, JS17b, LL13a, PNG10, RS12, RHPWS13, REL17, VHR16, Vik11, ZXS+10].

toolbox [HPT\textsuperscript{+16b}], toolchain [KSH\textsuperscript{+17}], toolkit [FSC\textsuperscript{+14}, GS12, IgK16, MJBM12, MSS\textsuperscript{+13}, MADWB11, NKJ16, PG15, PPM15, TS10a, ZLL\textsuperscript{+13}], Tools [RLG14, GMZ12, SLG15]. toolset [YPKB12]. topographical [KYG\textsuperscript{+15}].

Topological

Jan16, AR15, PRYI\textsuperscript{+17}, SB11, TSZQ12, VAR12, VBMA13, Wei12b, vSGP10].

topologies [Gar12, TSNC\textsuperscript{+17}], topology [AD10, ASS\textsuperscript{+17}, Dii15, FED17, GMSdG15, KP11, MSSP17, yOaCG10, Rod13, dCDP15, BLG10].

topomerization [GG10].

Topological

Jan16, AR15, PRYI\textsuperscript{+17}, SB11, TSZQ12, VAR12, VBMA13, Wei12b, vSGP10].

topologies [Gar12, TSNC\textsuperscript{+17}], topology [AD10, ASS\textsuperscript{+17}, Dii15, FED17, GMSdG15, KP11, MSSP17, yOaCG10, Rod13, dCDP15, BLG10].

topomerization [GG10].

Toroidal [SS13b]. Torque [Elk16].

torquoselectivity [GMBX\textsuperscript{+16}].

Torsion [DPSL16, FZY\textsuperscript{+12}, HP10b, HXM\textsuperscript{+16}, JMX\textsuperscript{+16}, YZ16].

torsional [BAS14, PRRT\textsuperscript{+10}], Total [BEEL14, IKN13, MA16, SM16a, WX12].

toxicity [TTB\textsuperscript{+11}, TTL\textsuperscript{+12}], TQ1 [VL17b], TQ1/PC [VL17b].

track [ENKK\textsuperscript{+17}, RHT\textsuperscript{+15}], tracking [BHR15].

tractable [KFY\textsuperscript{+13}], training [DBDP16].

Trajectories [AST\textsuperscript{+16}, HRID16, JZL\textsuperscript{+17}, KG13, LZS\textsuperscript{+17}, PSP15, RN17, SFR\textsuperscript{+11}, ZSS\textsuperscript{+13}, dSVdM\textsuperscript{+16}].

transcription [XMSZ16]. transform [Ano15-58, BH14, Ish12, LL13a, SZTSM10, YWJ\textsuperscript{+16}].

Trans [CSM16, MSBF16, BLS10], Trans- [MSBF16], Trans-2-Butene [CSM16].

Transformation [CCOH14, APY\textsuperscript{+16}, DLW12, KZZ\textsuperscript{+16}, REH13, RSK\textsuperscript{+15}].

transformations [HDL\textsuperscript{+14}, SJC11]. Transiting [CM13a].

Transition [OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JZ17, LYL16, LDZW17, LN15, LZW\textsuperscript{+11}, LGKS17, LLL\textsuperscript{+12}, MTM14, MS10, MN15, NMLD13, PHK14, RAGLL11, RJ\textsuperscript{+11}, SJJ\textsuperscript{+15}, VVV\textsuperscript{+15a}, YZGS14b, YWZ14, ZWW10, Zim15].

transition-metal [LDZW17]. transition-state [CSAdOM17, RAGLL11].

transitions [AKK\textsuperscript{+16}, BD11, DH11, HS17b, Hb15, MCvdV13, PBDW11, SBT17].

translationally [MRO17]. translocation [MJC14]. transmembrane [DSF17, LMI\textsuperscript{+14}, LAW\textsuperscript{+16}, WXL\textsuperscript{+12}]. transmission [LLJ12].

transphosphorylation [WXY14]. Transport [DJX\textsuperscript{+11a}, DMN15, CWHH11, CBTZ16, DMN14, DJX\textsuperscript{+11b}, HLWD15].
LHO17, LJ012, NS17, PGG15, SLI12, SY16b, TCX13, ZYG15.
transportation [LYZ12a]. trapped [DM15, VIT15, WLW10]. Treating
[PLCA17, SMP17a]. Treatment
[HSH15, CGOA17, GPK12, Has14, HGH14, MG14, NS10, Sch12, SSWX14],
[CXS10, PH15, dSdLB16]. tri [ZP13]. tri-N-acetyl- [ZP13]. triad
[LY10, SM16a]. triadic [PPUB16]. triads [YKH10].
triaminoguanidinium [ZYL12]. triangles [She12]. triangular [TS11].
triangularly [LWZ13]. trimethylsilyl [BM11]. trimethylsilyl [GL16].
trimetallic [GLF16]. triethyleneglycol [GL16]. triethylgermanium
[WHX10].
triethylenetriazine [RA09, Gav12, GRD15]. triazenes [YPC10]. triazol [ZWT12].
triazole [NS10]. triazoles [GKR13, Ray13, RKG11]. trichlorostannate
[PKK17]. tricyclic [VSD10]. triel [YKH15]. triene [ABD12].
trifluoroethanol [JA10]. trifluoroethanol/water [JA10].
trifluoromethane [CLC11]. trifurcation [HOM16]. triggered
[DA15]. triggering [LDD17]. trigonal
[Ano11, Gav12, GRD10, JHMB09, JHMB11]. trihydride [PM13].
trimer [THP15, YCA10]. Trimeric [PMT16, RCM13a, RML15].
trimetallic [GL16]. trimethylsilyl [BIL10]. trinitrotoluene [SH14].
tripeptide [BH15, GOM16]. triphenylamine [MSV16].
triple [ACD13a, ACD13b, POB13]. triple-zeta [POB13]. triplet
[BS17a, THP15]. triplets [EK15]. tripodal [SB10].
[FP10]. Trotter [VKAM12]. Trp [EJ13]. Trp-Glu [EJ13]. TRREAT
[CM13a]. truncated [CFE11]. truncated-CI [CFE11]. truncation
[ACD13a, ACD13b, CS14, MC12]. trust [PLA11]. trying [BRG12].
trypanothione [VSD10]. tryptophan [EOA11, PS14, SHB17, VMT10].
Tsalis [QZ10c]. TTTO [JW12, SLHW09]. tuberculosis [MPNS13].
tubes [TS15]. tubular [nLH11, ZLY16]. tularansis [STM15]. tumor
[AI11]. tuned [BK17b, HZS17, ZZS16]. tungsten [TS15a]. Tuning
[Ano11, JHMB09, JHMB11, BK17b, LWW11, Mor15, RLG11, WTY17, LZ12].
tunnel [KL14]. tunneling [CSAdOM17, HS16a, LZW11, OT12].
TURBOMOLE [KK17b, RR14, STH10, vW11]. tweezers [MA14].
twelve [Pog10]. twist [KTK17]. twisted [YLZ10].
Two [DS12b, KKN11, KTO13, SC17, COH14, DBP12, ECZ17, FSA14,
GAMAC14, HLH12, LPS11, LRER13, NASH15, PS17, PW12, SL14,
SJC11, TCP14, VT14, YAS13, YLL11, ZTH15, SM17].
Two-Body [SC17]. two-center [LRER13]. two-component [NASH15, PW12].
Two-dimensional [KTO13]. two-electron [PS17, YLL11]. Two-level
[KKN11]. two-photon [DBP12, ZTH15]. two-scale [FSA14].
Two-step [DS12b, SJC11, TCP14]. type [BM12, BE16, CYY17,
CRC13, CB11c, DI15, HLH15, JYC16, LH14a, MY17a, MY17b, MK15,
RKB14, SZX13a, SZX13b, VED10, WvRSM14, ZK11]. type-II
[CB11c]. types [SKY11, UT15]. typical [TZ12]. typing [FP17b, YPK12].
uranyl [OSS10]. URBOMOLE [BBG\textsuperscript{+11}]. ureas [FCL\textsuperscript{+10}]. ureido [SSP\textsuperscript{+13}]. ureido-benzensulfonamide [SSP\textsuperscript{+13}]. uridines [DPSL16]. urokinase [BM12]. uroporphyrinogen [BEL\textsuperscript{+11}]. uroporphyrinogen-III [BEL\textsuperscript{+11}]. Use [DCOD13, GPM17, HCD\textsuperscript{+10}, MPA12, MMZW14, NPTS16, NC14, NDD\textsuperscript{+10}, RL12, WM17, Yes12, BCP\textsuperscript{+10}]. used [PGY15, Pie14, PLAG11, TH13]. useful [SMGB11]. usefulness [PSP15]. user [All11, DBF14, HH16b, JJW\textsuperscript{+14}, LBB\textsuperscript{+15}, PVZ13, SFR\textsuperscript{+10}, STH\textsuperscript{+10}, WPM\textsuperscript{+15}]. user-friendly [SFR\textsuperscript{+11}]. users [GKV\textsuperscript{+13}]. uses [BCJC\textsuperscript{+14}, FHMB15]. Using [BS15, Car14, DLL\textsuperscript{+10}, HH10, HPSK12, LLvG10, LG14, MP11, QLQ11, SK17, TNG\textsuperscript{+10}, WF16, AASP18, AG11, AGM\textsuperscript{+13}, AC12, BW11b, BMR11, BDP11, BB11a, CVT\textsuperscript{+11}, CAP17, CSSB11, DWL11, DBK17, DFF\textsuperscript{+15}, DCHL12, DLZ15, EWK\textsuperscript{+13}, FF11, FLM11, FL15, Gar12, GR15, GFPSD17, GMO16, GZM11, GRL\textsuperscript{+11}, GRL\textsuperscript{+12}, GMBX\textsuperscript{+16}, HASR\textsuperscript{+12}, HNS16, HLW\textsuperscript{+17}, HDL\textsuperscript{+17}, HH17, Höf14, HBL12, HYUS11, HJKJ13, HZSS17, HHWL17, Hug14, HRH\textsuperscript{+17}, Ish10, IHJ\textsuperscript{+13}, JLS13, KV13, Kan15, KERY\textsuperscript{+16}, KT10, KLOS10, KTNN10, KP11, LBGS16, LPK16, LRvdSM15, LZ12, LCH10, LCL\textsuperscript{+10}, LMR14, LHG11, LTA\textsuperscript{+11}, LBDP12, MS17, MZZ11, MRB14, MJ14, MN15, MY17a, MSS\textsuperscript{+13}, MKM\textsuperscript{+17}, MUCJ15, MKVS10, MKB\textsuperscript{+13}, MFR\textsuperscript{+17}, MIOM13, MMJ10, MS15, NLP\textsuperscript{+16}, NASH15, NH11, NOC\textsuperscript{+15}, PGd0\textsuperscript{+16}, PC11, PG15, Pie14, PJ13, RB13a, RLDJ17]. using [RDDS10, RJH11, RS13, RRR14, Ric16, REL17, REV\textsuperscript{+17}, Rui11, RFH10, REH13, SHMO11, SFM14, SDF\textsuperscript{+17}, SBV10, SA13, SCW11, SEF\textsuperscript{+16}, SHL\textsuperscript{+11}, SKKS13, SY11, SRS14, SZSS16, STS15, TYZ\textsuperscript{+16}, Tak14, TKNN10, Tsi17, TJB12, UTM11, VKAM12, VECT12, VI17, WKLC12, WdVN12, WLC12, WZ17, WJX\textsuperscript{+10}, WDZH13, XTY\textsuperscript{+14}, XYX17, XWW\textsuperscript{+11}, YWJ\textsuperscript{+16}, Yon16, YN15, YDX16, ZWLX11, ZL11, ZLT13, ZWS\textsuperscript{+10}, ZP13, ZH12, ZHHX11, dLC17, LHL\textsuperscript{+10}]. utility [YHVM12]. utilizing [BVY\textsuperscript{+12}]. UV [GGM\textsuperscript{+12}, KASH14, RDF\textsuperscript{+11}, RVdMB16]. UV/photoexcitation [RVdMB16]. UV/Vis [GGM\textsuperscript{+12}].

V [WWKS16, LZL\textsuperscript{+15b}, MG11, PBE16, WRM\textsuperscript{+12}, WYGW12]. valence [FF11]. Valence [WM12, YWZ14, BEEL14, BACSCJ\textsuperscript{+10}, FE14, GCW16, Hill13, HAI\textsuperscript{+16}, lbr17, KGR\textsuperscript{+16}, LLW12, LWJ12, POB13, RHRCH16, Rx112, SMW09, SCSW13, TM16, WWU12, XP13, XhD15, vLBBR12, GWF11]. validation [GMMH\textsuperscript{+16}, GCP\textsuperscript{+13}, PFV14, WMW\textsuperscript{+10}, ZST14, G MG\textsuperscript{+10}, HM13]. validity [LP11b]. value [SG10a]. values [BA11, GKi5a, SK12, Zha12b, Zha12a]. vanadia [GNCA10]. vanadium [WYGW12]. vapor [BDTP11, SISK10]. variable [KDB13]. variant [TKT11]. variants [SLY\textsuperscript{+10}]. Variation [IMK\textsuperscript{+16}, Lvg13a, MTvG12]. Variational [RAGLL11, TH13]. Variationally [YK13]. variations [LLHM16, SH15]. various [CC11, DSM\textsuperscript{+11}, GVP\textsuperscript{+10}, GMO16, MJBM12, PGC12, PL18, SOYC12, WDW12]. varying [CC12a, GC11]. VASP

W4 [KSM17]. W4-17 [KSM17]. Waals [BLF14, BB11a, BC13, CR14, DS12b, DSF17, KBC12, KCK+15, KGHK12, KLN12, LCH+15, SMGB11, SLIB12, SJZ+15, SYZ+17, YZZ+17, ZY14].

water-fluoride [NC12]. water-halide [NC13]. water-vapor [SISK10].


Wave-function [HH16a]. wave-functions [Fer13b, Fer13a]. wavefunction [FD16, GSS13, HPT+16b, KSH+17, LC12]. wavefunction-based [GSS13].

wavefunctions [Bar14, BWKW10a, BWKW10b, LP11c, MDTD13, SAGC16]. Wavelet [WRHF10, PN13]. wavelet-based [PN13]. waves [TCB16]. ways [KV15a].


Web-based [Gar12, JIW+14]. web-user [WPM+15]. WEGA [YLGX14].

weighted [Fer17, HNS16, HHWL17, LMZ+11b, PRY1+17, RHH11, ZH12, Hill13]. weighting [WDHI13]. Weinheim [Spr10]. well [CME11, LrE17].

dell [LrE17]. wells [GKSS14]. were [G16, MFEM16, XFG+16].


Wiley [Spr10]. Wiley-VCH [Spr10]. Window [DAB16].

Window-Exchange [DAB16]. wires [LZY+12a, NS17]. wise [KSS17].

withdrawing [CWHH11]. within [AIGP15, BBG+18, CKL+11, DVPV14, GL16, HKR+14, IHI15, Lar12, MKH+13, RCM+13a, RML+15, RHPWS13, SFCCK+14, SFCX+15, SFG+17, Sch12, SJ+15, WC11, WPM+15].

without [FSD+18, GA14, KJ10, TH13, dLC17]. Wolf [GPSS12].


X [ASS+17, CXS10, GKP+16, EPH+15, LDJ+10, LLL+11, LZJ+11, Li14a, Li14b, LGW12, LCWW10, LWD13, PMG+16, SPS+12, SZBM13, SLIB12,
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TFQ+11, UT15, YS13, ZYLL12, ZLLL12, FZY+12, FLM11, JJ16, Kop15b, LLBO12, LHS12, Lz151b, LCW10, PDG+16, SKY+11, WWD14, XML+15, XhD15, ZLLH12, LX11]. X- [SKY+11]. X-ray


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Anonymous:2016:IIITa


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Anonymous:2016:ITe


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Zalesny:2015:TAD


Zuev:2015:NAI


Zhou:2017:BHH

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