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Title word cross-reference

(Φ, Ψ) [WD04]. (φ, ψ) [TTB01b]. −2 [ZZZ+06]. −4 [ZZZ+06]. 1 [FROD08].
1/τ [SG01]. 12 [KGL07]. $139.00 [Sta00]. 14 [LMGR06, ZGXX06]. 16
[HXD08]. 2 [DMC05, GdAcV+07, LW04b, LXZ06, LW06, PF06, SFC04,
WDZS07, YNW05, hYDN+08, ZTS09]. 2 ≤ N ≤ 372 [Pul05]. $3 [Lip00]. 3
[BAH+02, FROD08, GDPCPU07, GdSuM+07, HP05, mJzL+08, KSN01,
LYZ+08, MP03b, PF06, SHBD05, SFC04, TJM+03, WLL07a, WDZS07,
XLL+02, ZLY07]. 3_{10} [JS07b]. 3d [Hol05, LD05a, Wu06, SZT08]. 4
[FFH+01, LLXS02, QB05, WDX+02]. 4, 7 [ZWS+02]. 4d [ABYM08]. 5
[ZXL+04]. 5d [HZ09]. 6 [Han01, LLXS02]. 7 [LMO09]. 8 [KS05a]. 9 [UM03].
[n] [VKP+08]. ## [BRV+07]. +
[FKS+09, GLRL02, GPSP06, GWL07, HDO+02, ITS06, KT08, LMO09,
Mck07b, PV07, Sha02, WWT08, ZWY+09, ZL05, dRLMS00]. +2 [PNG08]. −
[Bac09, Dib05, HTN03, LYZ+08, Mas01a]. 1
[AGI+07, IS03, LDT+02a, XZ04, ZX04, ZLLS04b]. [HWFN01]. [FHR+01, VBS09, ZLD09]. [LKA01]. [FO04]. [Σ] [BAL+01]. [Σ]/ [BAL+01]. [2] [BAL+01, Gog08, PRSM03, ZWS+02]. [2+] [AS06, BTP09, BL00, FHRR07, GSPS06, HLB09, KRLD09, Kri08, ROG00, TFZRG01]. [2-] [IvSV06, JD09]. [2π] [Gog08]. [3] [BPC01, LDT+02b]. [3+] [BTP09, BL00, Kri09b]. [V] [WC08]. [57] [HLLN06]. [a] [VBS09, CJW+09]. [Mu05], \( IS^2 [Bac09], \) \( \text{MTCP1} [BRDC02] \). [ZZZ+06]. [p+] [GPSF06]. [0] [DLD+02]. [1] [BPC01, LDL+02, WLPF05, XWXC08, YK09, ZZ09, XWXC08]. [103] [NS0+07]. [11] [XB08]. [12] [WZZ+09, XB08]. [141] [GYCZ04]. [18] [ZZZ+06]. [2] [Bac09, BAL+01, BL00, BBI+09, CPJ00, CCCJ09, CTFC08, DLD+02, DRAS04, DRAS05, Dib05, DMM05, Dom08, FJ08, GCCVB00, GDP05, GSPS06, HYR06, HK07, Hua09b, IN08, IV04, ISV06, IS03, JFF+00, mJLZyL07, KZY09, KS05a, KKJH08, KBL08, KS05c, LDM01, LC07, LWK08, LLXS02, LW04a, LZZC09, LAT05, LF02, LDT+02b, LWY+09, LMO09, MR02, Mas01a, Mas01b, MGLL03, Mdc08, Mck07b, MY08a, NA06, NYHN06, NHH06, Owe05, PGNG03, PGRN03, PC00, PRSM03, PL08, RAGL09a, RAGL09b, RD00, RDM+08, SLL+04a, SLL+04b, SRE08, STC+08, TJM+03, TD08, UTC+03, UTT+04, VS02, WLLS05, WDS06, WDS06, WLL07a, WDD07, WLL+07b, WD08, XFD06, YTY07, YLYW+08, YLYL09, ZY01, ZZL04, ZLLS04b, ZWL+05, ZLLS06a, ZLLS06b, ZKZ+07, ZX03, ZX09, dOMS01, dRLMS01]. [20] [Ber03, CCB04, Ell07, GB02, Var09, WLPF05, WL09b, ZZZ+06]. [+] [dOMS01]. [2] [LMCD09]. [2+] [GHLK+02]. [2+] [GYM07]. [2A] [YK09]. [3] [BPC01, CPJ00, DRAS04, DM05, FJ08, GDP05, G06, HLLS05, HYA02, HDO+02, HT03, ITS06, mJLZyL07, mJLZyL08, KZY09, KT08, KKJH08, KSTC01, LDM01, LD05a, LMK01, LDC+07, LW04a, LWW+06, LF02, LWY+09, MR02, Mas01b, MGLL03, Mck07b, Mui05, NA06, ON07, PGNG03, PGRN03, RDO0, SAS05, SLL+04a, SM06, SC08, TJM+03, TK08, TD07, UTM+02, UTT+04, VDM06, WDS06, WLL+07b, WD08, XDS06a, XFD06, YLYW+08, YLYL09, ZIM+07, ZZZ04, ZLLS06a, ZZW+07, ZZ+08, ZXYF09, ZZZ+09, ZKZ+07, ZWS+02, ZX08]. [3-n] [mJLZyL08, KSN01, WLL07a, WDD07]. [3] [CS01]. [4] [DRAS04, DM05, IN08, IV04, JD09, LDM01, LM01, Mck07a, PHH+08, TYN05, TK08, UNM+01, UTM+02]. [4-n] [FHR+01, WDX+02, XL+02]. [5] [GD06, LY+08, SLL+04b, ZLL04, XWXC08]. [50] [ZZvRSC08]. [54] [GZ07]. [6] [BS01, GHLK+02, Han01, KRLD09, LDM01, LZZC09, LAT05, LY+08, RPJ07, SLL+04b, TY05, XB08]. [6-n] [Han01]. [60] [CJS+03, Ell07, KJP+07, Owe05]. [62] [HK07, STC+08]. [64] [CTFC08]. [4-] [CTFC08]. [7] [HYA02, LZZC09]. [s] [GZ07, Mck07a, Mck07b, PLC08, WLL01]. [80] [KSN01]. [9] [Mck07a, Mck07b, PLC08]. [90] [NS0+07]. [A] [Sha02, KKS04, MK02, ZPL07]. [cam] [ZAT07]. [carbene] [HA04]. [h] [WLPF05]. [i] [OS08]. [m] [LY+08]. [N] [BP01, BS05, HT03, MG00, Owe05, RC04, YT04.

/As [KS05a]. /CBS [Lu09]. /CCI [ZLLS06a]. /CF [YLWL09]. /Cs [GLRL02]. /empirical [CYM02]. /free [BG00]. /Ge [LLXS02]. /GeH [LLXS02]. /Mn [BL00]. /poly [BSJ01].

0 [Bic09, CG06, Lip00, Sta00]. 0-470-03735-0 [Bic09]. 0-471-33135-X [Sta00]. 0-471-96588-X [Lip00].

1 [AJNG01, AVS09, BPC01, BWE05, KF08, NLL+09, SPT+03, VVS07, WC09, WH08, YT04]. 1- [CUS00]. 1-aminoo-3-propenal [FDSA00]. 1-jk [SPS08]. 1-naphthoic [CMLS05]. 1-pK [ZCS04]. 1-x-bicyclo [BPC01]. 1.0 [AGSFA+05]. 10-endoperoxide [CG08]. 10-membered [ZW09]. 1174 [WWC+05]. 12 [HDO+02]. 12-crown-O [HDO+02]. 1291 [Ano06a]. 1328 [Ano05b]. 142 [Ano06b]. 1629 [WB04a]. 1Z [Lu09].

2 [BL08, LBG08, MM02, PFR04b, Håf05, HTN03, MG00, PO03, RC04, WC09]. 2-allyl-2 [ZGZX07]. 2-aminoo-2-imidazoline [XKG+05]. 2-amino-2-oxazoline [XKG+05]. 2-amino-2-thiazoline [XKG+05]. 2'-aminoarabinonucleosides [BL08]. 2-Aminopurine [SC01]. 2'-aminoarabinonucleosides [BL08]. 2'-azido-2'-deoxyribonucleoside [PFR04b]. 2-chloro-[JMK08]. 2'-deoxyguanosine [MM02]. 2'-deoxyribose [LBG08]. 2-difluoroethane [CUS00]. 2-dihaloethanes [WFR08]. 2-dihydro-pyrimidinyl [WJX+08]. 2-dimethoxethane [LCGA03]. 2-electron [ABF+03]. 2-H [LDC+07]. 2-oxazolidones [OY01]. 2-oxo-1 [WJX+08]. 2-oximidazoles [JMK08]. 2-phenoxycarboxyl [XKKL03]. 2-substituted [OSA06, WW04]. 2-thioaracil [LMGO+09]. 2.0 [GZM09]. 21C7 [GLRL02]. 21D8 [UTH+03]. 22 [Bof01, Qua01]. 24 [Ano06b]. 25 [Kne05, WB04a, WWC+05]. 26 [Ano05b]. 27 [Ano06a, Ano06c]. 28 [HNWF12, Van08]. 2B6 [LCC09]. 2B6-substrate
3 [AAP00, KAK+09, LEV+09, NYTH09, Rud05c]. 3-butadiene [Hir08, WR07]. 3-dihydroxy pyridine [YXZ+04]. 3-dimethylallene [ZPL07]. 3-fluorobutanal [NSB08]. 3-hydroxy-2-mercapto pyridine [YXZ+04]. 3-trimethylisilyl-1-pyrazoline [LLKC06]. 311 [Wib04]. 31G [BRV+07], 3IG* [RRP+01, FKJ+01, NL08]. 3IG** [WD04]. 31G*/AMBER [FSFK05]. 34 [PHH+08]. 3a [HKHN08]. 3D [DHW+08, SGPS09, CGMPT+08, CPUGD09, MH08b, VB09]. 3D-chiral [CGMPT+08]. 3D-RISM [MH08b]. 3D-structure-function [CPUGD09]. 3DEX [SHBD05].

4 [Lu09]. 4-carbonate [vDSSvA04]. 4-dihydropyridine-based [HSMT04]. 4-dimethylamino-benzonitrile [ZH08]. 4-dithiacyclohexane [FD03]. 4-dithiane [FD03]. 4-Spinor [PV03]. 43C9 [CBS+03]. 45-ns [SO07]. 4d [CWWS07]. 4R [BISB02]. 4R-hydroxyproline [BISB02].

5 [LDY+08, PFR04b, PMM05, TAS07]. 5-di-tert-butyl-o-dimino benzosemiquinonate [Bac09]. 5'-diphosphates [PFR04b]. 5-hexadiene [PA05]. 5-hexadiyne-3-enes [PWFS01]. 5-hexatrienaldehyde [ZGZX07]. 5-nitro-3-carboxy benzisoxazole [UTH+03]. 5'-phosphate [PMM05]. 5'-phosphate-dependent [LDY+08]. 5-phospho- [RGP+07]. 500-MHz [CMD+04]. 53A5 [OVMV04]. 53A6 [CLWL09, OVMV04].

6 [BRV+07, Wib04]. 6-311 [Wib04]. 6-31G [BRV+07]. 6-3IG* [FSFK05, RRP+01, FKJ+01, NL08]. 6-3IG** [WD04]. 6-bisphosphatase [MRS+07]. 67-residue [MH09]. 6G [VSW+03].

7-species [WG02]. 790 [Ano06c]. 7a [HKHN08].

8-nitroguanine [JM07a]. 8-oxoguanine [FPN+05, JM07a, Pin03].

9-heterofluorenes [CZF07].

= [Bac09, CPJO00, CRC+08, GHLK+02, GSPS06, Han01, HT05, HYA02, HKHN08, HZ09, Hua09a, JJK+00, KBL08, LS08a, LZZC09, LYZ+08, Mar03, Mc07a, Mc07b, OS08, RBO1, STC+08, WLLS04, WZZ+09, WD08, WWS07, XFF06, ZJM+07, ZY01, ZXY03, ZL09b].

A*0201 [WCF04]. AA [KB02, KDSV02, POJ01, PB05, XLT07]. AA/L [KOML08]. Ab-initio [Haf08, HELM09]. abasic [FPN+05]. ABEEM [YZ06]. ABEEM/MM [YZ06]. abilities [OYH09]. Ability [GM01, RRZA08]. ablation [KZW+05]. ablation-mass [KZW+05]. ABO
[WD08]. **ABSINTH** [VP09]. Absolute
[BWE05, ZM09, BMRF01, DHF+05]. absorption
[MWL+08, MSH+06a, YXZ+04]. abstraction [AST06, CUS00, CUSS03, GAIMVB01, mJiZLyL07, LW04a, LLL07, TGLL07, WLLS04, XLL+02]. Ac [GHLK+02]. accelerated [Gou07]. Accelerated
[LSG06, LDG02, FSM09, Har04]. Accelerating [FEV+09, LEV+09, SPF+07]. Acceleration [KG02]. accelerator [ATMK03]. acceptance [KBB09]. acceptor [BL06, RM07]. accessibility [AG03, ENM+04, GP06, Tot04]. accessible [BHW00, BMLV04, GB04, HHS+05, LFBSK07, RP07d, TSMNG01, TRS02, ZCL09]. accessible-surface-area [ZCL09]. Accompanying [Ish02]. account [May07, SN06, Vya01]. Accuracy [FII+07, GG09, PSMB05, SKK+07, UBFP04, JS07b, KC01b, MKGA06, MH04, RK05, SM03, SW06]. Accurate [ABWT09, B4PMRA100, EK06, GK09, Gri04, H06, H06, HMS06, Ish04, LLZL09, MSH+06a, Tot04, WFHP01, WHP02, WHF08, WX09, ALKH04, Bie04a, BLB09, CGBF05, CF06, GKK07, H06, SM05, JJK+00, Rud05a, Rud05b, Rud05c, Vas02, WCC08, ZF08, vEM01]. accurately [IGL07, SBI08]. acetaldehyde [Lu09, YLZ08, Lu09]. Acetalization [RUPH06]. acetals [MG06]. acetamide [CCK01]. acetate [GWM08, PGG06]. acetic [MH08a, YT03]. acetonitrile [ELK+09, GJK00, NL07]. acetylcholine [GCD+08, MCK05]. acetylcholinesterase [MCK05]. acetylcholinesterase-catalyzed [MCK05]. acetylene [LDL+02]. AcF [GHLK+02]. acid [CJK+02, CML05, CJK09, CCK01, DP03, DP04, DLHC06, DHH+07, FZL07, HFHL06, HLC09, IT03, IJK09, JF00, JKM08, JCL05, KLBO3, LL07, MT03, MMLC05, MSF+08, MH08a, Nak07, NH05, NLL+09, Pac06, RR05, RKK03, SKGS00, SY03, SL04, SGB99b, SWR06, SHK+05, UNHYT06, VM02, XISH06, XLC08, XL707, YT03, YXL+09, ZZ070, ZY08, ZOJ+06, vDSSvA04]. acid-3 [vDSSvA04]. acid-catalyzed [RRO5]. acid-nucleotide [MSF+08]. acidity [ELK+09]. acids [BE06, CADW03, CLA+00, FM00, HTL03, HP04, IJK09, KSO1a, LDV+08, MB00, MM05, NH05, OM01, PM05, PPYS08, Van02a, XKKL03, YLL+09, ZLD09]. AcO [GHLK+02]. across [HZX04, SS08, SRB06]. act [GM01]. actinide [AB00, GHLK+02, NS0+07, VMA03]. Activation [EL06, BGC+09, BZL05, CC09, CF04, KT08, Lu09, PV07, RRS06, Vya01]. active [AG00, BSDM04, CFR06, CFS+09, FCP+04a, FCP+05, HBM06, HFS+07, HYR06, JHPRSM+05, KSK00, KZ00, LLL03, MDA08, PDM06, RZWS07, SSO5, SFR07, TDB06, XL08]. active-site [SFR07]. activities [HMM809, MS04, ZWB09]. activity [AGMPRG+08, Boun01, CW02, DD08, DA01, DHH+08, DHH+09, FTL01, GDPP08, LC09, MRS09, Sha02, WZY04, Zer08]. acylation [MCK05, MK02]. adaptable [KF08]. Adaptation [HLM05]. adapted [FCP+04b, H06, H06, LX07, PTC01]. Adaptive [BHW00, HBW01, HW03, HLSH05, DK01, GY08, OM04, RNG03,
SJJ+04, WCS09, LS08c]. addition [BLO+02, DGD+05, LL00, Mui05, RAGL09b, RR05, WCW08, WSC09]. addition-elimination [Mui05]. additions [AVB00]. Additive [GGK+08, CCK01, LKA01]. adenine [KKMMS04, SG07a]. adenine-thymine [KKMMS04]. adenosine [MRS+07, YKK09]. ADF [tVBB+01]. adiabatic [SLRC01, TVL+03]. ADMA [EM03b]. admissible [WG02]. adrenergic [YKK09]. adsorbate [BWI+02]. adsorbed [DR09, PBZ00, XPW09]. Adsorption [ATH+03, BRS00, BRS01, HSF08, ZTP+08, NK06, SURG06, ST04, WLX+05, ZCS04, ZSC05]. Adun [JGVF05]. advanced [LAEL01]. advances [MMRVH07]. Advancing [PP08b]. aect [AST06]. anities [AVS09, DJ04, KS05a, KKMMS04, LLXS02, MRS+07, SRB06, WSM+08, ZJM+07, ZXL+04, dSGCG00]. anity [ABA04, FO08, GCD+08, KFB05, KS08, Lee09, LXW+09, MML+06, RTG00, SOOF05, SWV+05, ZBW09]. affording [OY01]. after [TJM+03]. Ag [GPSP06, LYZ+08, NA06, SG07a, WCS09]. against [SSS+09]. AGBNP [GL04a]. AgBr [Sha02]. agent [LHJ+06]. agent-based [LHJ+06]. aggregate [KHF+09]. aggregates [AB08]. aggregation [IM06, OGH05]. AgN [ZX08]. agonists [GCD+08, SBG+09a]. Agreement [LS05b]. aided [PPJ+07]. AIM [SFC04, CFSo3, WW03]. AIM2000 [Ano01a, BKS02]. AIM2000-Program [BKS02]. Al [OS08, WZZ+09, Van08, KKJH08, QB05, WZZ+09]. al. [RKH03]. Ala [PC00]. alanine [DSR+07, ECA06, GAIMVB01, GSBO9, GKTSo4, HHP04, HKM02, JW06, LSW+01, MOP+07, MFR07, PFJ+03, Quao7, WD04, ZW09, ZM06]. albicans [RGP+07]. Alchemical [Blo04]. alcohol [FBDG06, JHMB+09, JHMB+11, WWT08, ZWY+09]. alkali [BSG07]. alkaline [JHMB+09, JHMB+11]. alkaloid [BMRF01]. alkane [HGMB04]. alkanes
alkyl [BE06, CC07, EB04, LLZL09]. alkyl-cyanobiphenyl [CC07]. alkylation [EL06, VBGL+00]. alkynes [W CW08]. All-atom [FM00, MB00, VGO+07, GB04, IT03, MT03, PHH+08, RG08, WS07, JS07a]. All-electron [EL09, ITN+05, IS07]. all-purpose [JGVF05]. all-siliceous [LST08, LTV08]. allene [WCHW09]. allenes [WCHW09]. allocation [SKSH07]. allosteric [LGB+09]. Allostery [Sen06]. alloys [GD09, KGD06]. allyl [ZGZX07]. AlNC [MLCD01]. alpha [GKK07]. Alpha7 [GCD+08]. AlPO [PHH+08]. altered [DLRZ09]. alternating [YFR05]. alternation [JPCA08]. aluminophosphate [LMV07]. aluminum [TBG00]. always [Kol04]. Alzheimer [MS03]. AM1 [DC02, FRS05, JBJB00, JJB02, LMMW04, RFSS06, TCT03, VGGMM05]. AM1-BCC [JJB00, JJB02]. AMBER [Ano06c, WWC+05, CCD+05, FSFK05, JS07b, JM07b, MRC03, OYH05, TdMSD+08, WCC08, WCC+04, WZW+06, WS07]. AMBER* [CLA+00]. AMBER95 [ONHN00]. ambiguous [BS01]. Amica [GBL+05]. amide [CG03, CS01, CCP04, CSRST04, CA07b, DDKV07, DRAS04, DSR+07, ECM+03, FK07a, FC06, FSS00, Gly06, GS07, Gra07, GHBB04, HHWG08, HS00, HSH05, HP05, IN08, JPF+00, JMD+02, JFG04, KB02, KK08a, KMH02, KSU03, KN04, KSK00, KMA+07, Kni00, LRI+02, LS05a, MGCA07, MS03, MWE02, MH04, MMP+07, MA05, NK06, NSU+02, OML+00, ON07, PFC03, PGH+04, PP08b, PYEA03, PAS07, PYCD03, PYS05, PC07, PLC08, RMHK03, RS07b, SH09, SMGE08, SSHT03, SFC04, SCF+09, SvDS01, TYN05, TCR+02, TT01, TD06, TTB01a, TTB01b, UTH+03, VGB08, VKCK09, WRBV03, YNW05, YK08, ZSE08, Zer08, ZWB09, ZHH09, ZB07, NYK+09, Ru07, VB09, RS07a, VB07]. analytic
[ASWG07, DOSG06, GL04a, IK00, KBT03, LFSB03a, LFSB03b, SJW09].

**Analytical** [HNWF07, HNWF12, PDC+08, QCK01, QCK02, RLR+04, WL02, DSR+07, HC08, HHS+05]. **analyze** [AGMPRG+08, Ham07, MCF07].

**analyzing** [DW08, LD05b]. **anradite** [ZWTP+08]. **anesthetics** [TZX01b, TZX01a]. **anF** [Han01].

**Angle** [Bof01, Qua01]. **angle** [CIB05, FWH+07, LI07, OFIK09, YL06]. **angles** [AGMPRG+08, Ham07, MCF07].

**anharmonic** [BP07, DB07, GBDP05, LMO09]. **anilido** [GTC06]. **anilido-imine** [GTC06].

**AnF** [Han01]. **AnG** [Bof01, Qua01]. **angle** [CIB05, FWH+07, LI07, OFIK09, YL06]. **angles** [AGMPRG+08, Ham07, MCF07].

**anticancer** [BZL05, PFR04a, SMM+08]. **antifungals** [GDPP08].

**anticancer** [BZL05, PFR04a, SMM+08]. **antifungals** [GDPP08].
XWC09, XKKL03, YS00, YK08, ZS04, ZS04]. Approached
[LL07, XSHC06]. approaches [BP07, Con02, CSD05, COL+06, MLJ03, PSF+08, PMM05, RLD09, RS09, SM08a, YCW+09]. appropriate [Bac07].
approximate [Cu08, GB04, Hol05, KS02a, SZT08, SYC03], approximated [PSF+08]. Approximately [EA06]. approximating [MR04].
approximation [AB09, BRS00, BR501, CLP+05, CCK01, Der09, EA08, GMA04, GWS+02, ION07, Kri09a, Lai07, LFSB03a, LFSB03b, LN01, MTC04, Nee03, OCB02, RP07d, SHSF05, ZFL+05]. approximations [Dya02]. APS [CBC+08]. APX [ZJM+07]. aqua [RMP01]. aqua- [RMP01]. aqueous [BISB02, CPJ00, CPJ01, CW02, CCK01, DA01, EK06, FHRR07, HMWC03, HRR05, HDO+02, IV04, IvSV06, JM07b, KEH+02, KPR04, Kri08, Kri09b, LRI+02, LR03b, Loe03, LMIF06, MM02, NL07, PK04, PHRR08, SH09, SMKM00, SBB02, VP09]. arabinonate [RGP+07].
arabinonohydroxamate [RGP+07]. arbitrary [KH06, LMV07]. architecture [TDK07]. architectures [TYO+02]. area [GCD+08, GB04, HHS+05, Lab08, LFBSK07, RP07d, VP02, ZCL09]. areas [BHH+09, TRS02]. arene [FKS+09, PCMG09, RRZA08]. arene-containing [RRZA08]. arginine [CJPZS08, SMGE08]. arginine-bound [CJPZS08]. argon [BWW+08]. argument [Ish04]. ARIs [PS09a]. arising [CCSJ00]. armed [KLM+09]. ArOCs [ZGXX06]. Aromatic [CPML08b, POC+07b, Van08, Bor03, FVB08, HLC09, MM05, MMGM07a, ST01, SMV+09, TDK07, VS08, WFP01, XLT07, PCO+07a]. Aromatic-Backbone [CPML08b, Van08, POC+07b, PCO+07a]. aromatic-type [HLC09]. Aromaticity [BPCD07, FMP08, JHMB+09, JHMB+11, LWW+06, LTF+07, MMGM07b]. Array [FP07, ABF+03]. arsenic [ALC08, KS05a, ZXL+04]. ARTE [VB07]. ARTE-QSAR [VB07]. artifacts [CCSJ00]. Artificial [PS09a, RWBH09, dVB01, CLC03, Gol09, NINAT+07, TCSM03]. arylamide [VIP+06]. ascorbate [HBM06]. ASIC [NYTH09]. aspartic [ZZY08]. Aspects [HHBH00, MO01, BMRRD01, BR07, Sie01, TT02]. assemblies [DFGB09]. assembly [DPR05]. Assessing [IB04, FGR07]. Assessment [BP03, CCWH02, DGI+08, KS08, LWH06, SSS+09, WSM+08, CKMC04, FMP08, GT03, LLS03, SP05, GGT08, GHBB04, TFZRG01]. assignment [BB05, BMRF01, PR02]. assignments [PF06]. assisted [BA04b, KT08, WJX+08]. assists [BM07]. associated [SRR06, TT08]. Associative [ABYM08, NL08]. asymmetric [WR07, WFR08]. Asynchronous [GLP08]. atmospheric [GCCVB00, PGNG03]. Atom [RP07a, RM00, BPC01, BR04, BWW+08, CCK01, FM00, GWS+02, GB04, HLLS05, IT03, JSL07a, mJlZyL+08, LMK01, MT03, MB00, PHH+08, RG08, RS08, SSB+03, SBLK01, SLL+04a, TGLL07, VK06, VGO+07, WLL07a, WBSR03, WS07, WLL+03, YLWL09]. atom-bond [VK06]. atom-centered [SB+03]. Atomic [DVP+02, FDM00, AS00, Bac07, BS+C+01, BCNs07, B0S+06b, BK00, BLT03, BAA07, CN03, FS04, GC02, Ish03, JBBJ00, JBBJ02, KRM+02, Kau07, KS01a, KCO1b, Lab08, LMV07, LST08, LTV08, Nl09.
atomic-centered [TBSM09].

atomistic [CA04, IDMC09, KK01b, RPMP03, SPGS08, ZALMG03].

Atoms [YM07, YK08, ALTB08, AD00, ASS+02, BHTCG07, BKS02, BS03, CMJ08, CDS09, EdlVR+03, FS04, HSF08, mJZsL07, KGN07, KS02b, LDC+07, Mat03, NSo+07, RP07b, RP+01, RLR+04, RLR04b, SO09, SM+06, SFC04, Wil01b, WDX+02, XLL+02, PFB05].

Atoms-in-molecules [YK08, RLR+04].

ATP [FCP+04a, GS04].

ATP-binding [GS04].

ATP-dependent [FCP+04a].

ATPase [HLB09].

attachment [LBG08, XWXC08].

attack [CBS+03].

Attaining [Rud05a, Rud05b, Rud05c].

attending [HT05].

aug [Wib04].

aug-cc-pVDZ [Wib04].

Auger [OKE+02].

augmented [JCHS07, KDG+09, LFK05, MOP+07].

autoantigen [KVS+06].

AutoDock4 [MHL+09].

AutoDockTools4 [MHL+09].

Automated [CKMC04, LMO09, HR08, LR03a, MM03, VSW+03, MHL+09].

Automatic [CHMI05, WK01, AGI+00, AGI+07].

automatou [XWC09].

auxiliary [GKH05, JSHG07].

available [SCF+09].

average [TRS02].

averaged [CP08, PYCD03, PYS05, PC07, PLC08, SMAV00].

averages [Rap06].

averaging [BS+01].

avian [DLRZ09].

avoidance [WCFH02].

axial [BMRF01, CN05].

axis [OMNH08].

azaglycine [LKJ+04].

azide [MSR04].

azides [ZX08].

azo [PFR04b].

azole [SMM+08].

azole-bridged [SMM+08].

azurin [PMGL03].

B-B-DNA [Maz01, Pin03].

B-domain [JS07a].

B-spline [ALKH04].

B-splines [GLO4b].

B3LYP [CLP+05, FSFK05, HWGB01, NL08, TCT03, WC04, WX09].

B3LYP/6 [FSFK05, NL08].

B3LYP/6-31G* [NL08].

B3LYP/6-31G*/AMBER [FSFK05].

Ba [WD08, XBO8].

Bacitracin [Dra00].

back [BB05].

Backbone [CPML08b, GKK07, Van08, Adc04, Ano06c, AHGK09, CIWL00, HSWN01, KLS02, LKA01, MFB04, MLL08a, PC0+07b, SP05, WZW+06, YL06, PC0+07a].

backward [KMP07].

bacterial [Ano06b, CPM03, GSO4].

bacteriochlorophylls [LKT04].

bacterioheme [IN01].

bacteriorhodopsin [RG02].

Bacteroides [SDM02].

Bader [GHBB04, SKH07].

Baker [WB05].

balance [Ano06c, WZW+06].

balanced [PB05].

Balancing [CF06].

band [AJ03, JCA+02, ZZW09].

Baoshan [JW12].

bare [KT08].

barrier [CRGN07, KSTC01, LSG06, MG06].

barriers [DBM03, EL06, HFHL06, PBF09].

bars [MDI04].

base [CCK01, DP04, FZL07, HWT03, KKKMS04, MMLC05, MSF+08, MHS05, NL08, OY01, PG04, PSS+04, PSMB05, SKGS00, SG07a, SBL05, SC01, SYC03].

base-catalyzed [OY01].

base-pairing [DP04].

based [Adc04, ALTB06, ALB09, AB09, BdPRMAI00, BMRF01, BDW00, BMTS01, CGMPT+08, CRK08, CLZ+09, CLZX09, CFS08, CHA+07, CPUG09],
CMBC08, CRGN07, CA04, CSB^+03, DLW06, DMLI05, DHW^+00, DBB02, DDVD09, DHW^-07, DHW^-09, DWC^+03, FCK^+08, FCP^+04a, FCP^+05, FM00, FZL^+06, FRL09, GZL02, GRCD01, Gon07, GDPCPU07, GDPP08, Gra07, GAS04, HSTM04, HS07b, HLM05, HZ06a, HZ06b, HMOG07, IJK09, IRO3, JD09, JKI08, JGVF05, KLS02, KBA^+04, KK08c, KBK^+01, Kob03, KIM^+09, KZW^-05, KVS^+06, LFKL00, LHJ^-06, Leh06, LXZ06, LJZ^-07, LH05, LLM09, LM03, MLL06, MSF^+08, MSH^-06a, MBH^-02, NLL^-09, NMAT01, OVMV04, PS09a, PFR04b, PA05, PAS07, PRJ02, PF06, PRDS08, Pul05, QLHL09, Rao00b, RSE07, RSER09, RLDI09, RSN^+02, RKA^-09, RUPH06, RRS09, RSS09, Ruv07, SAM06, SKSH07, SGPS09, SPL^-02, SBB02, SE08.

based [SZW^-05, TTB09, Tot04, VSK^-04, VB09, VGDSU08, WL09a, WL00, WS07, WRBV03, XYN^-06, XL02, YWHZ03, YNW05, hYDN^-08, YJF06, YXL^-09, YKK09, ZCL09, ZLY07, ZLD09, ZWB09, dSR08]. basepair [BCP03], bases [CCK01, Nak07, RTG00, RKH03, SL04, WRP^-06]. basic [Rud05a]. basicity [EK06, Lee09]. basins [CFS03, MP03a]. Basis [AHK02, BRLS08, BRLS12, JJ^+_00, Wib04, ABF^-03, ALK04, Bac07, By06, BR04, BT00, BS05, BRV^-07, CMJ08, CRS05, Cuf04, CGSdST06, DMZT08, EA08, EdiVR^-03, EL09, FZL07, GKH05, HmSd05, Hs06, HD06, IO08, JSHG07, KK08a, LFK05, Lai07, LM07, LST08, LTV08, MV06, Mas04, MLL^-08b, MC06, MY08b, MY08a, NSO^-07, OBB05, PSC^+01, Pen06, PFJ^-03, PSM05, RRP^-01, RLR07, SSB^-03, SMN^-06, TSSGS08, VKP^-08, VB03, Var09, VKC09, WMGK07, WTKM06, Wei08, ZWP^-04].

Basis-set [AHK02, MV06, Pen06, VKC09]. BCC [JB00, JJB02]. be [HmSd05, Hs06, HD06, IGL07, STSF02, WC04, BP01, LWV^-06]. beam [BAL^-01]. bearing [NL08]. Becke [AAP00]. Becke-3 [AAP00]. Becke3-LYP [PDS01]. Becke3-LYP [PDS01]. BeH [PRSMV08]. behave [PB02]. behavior [Ama02b, Bac05, BIS02, LB05, OO04, RP07c, SBB05]. behaviors [LML^-00]. being [OCB02]. benchmark [Ano01b, BSB05, DGD^-05]. Benchmarking [Hol05, ZT08, WS07]. Bennett [KB09]. Benzdiones [AS01]. benzene [BE09, BRLS08, BRLS12, HT05, HRG07, IIN09, LWX07, Sch00, SG07b, ZTP^-08]. benzenes [PB05, WRP^-06]. benzo [GLRL02]. benzocryptand [WWT08]. benzodiazepine [SPS08]. benzodioxoles [MRS09]. benzoic [BE06]. benzonitrile [ZH08]. benzylideneaniline [BY06]. benzylpenicillin [DSS03]. Beowulf [BMDB01]. Bergman [PWF01]. Besalu [Bo01, Qua01]. Bessel [DBS08]. Beta [LHI09, BTP09]. Beta-hairpin [LHI09].

between [AD00, AZM03, BS03, CFC06, DRA05, EFQ09, FG03, FL07, FO06, FKM^-06, FKM^-07, GMW08, HPP00, HRBBK03, HFHL06, HN02, Hri08, IIN09, JPC08, KWK^-01, KWK^-02, LDC^-07, L01, LL01, LFZS04, LLL03, LS05b, MST^-08, MBH^-02, OY01, PSF^-08, PMPGP05, PS03, RLR01, SM08a, SBLK01, Sim07, SWM04, SKK^-07, SP05, TY05, TK08, TDD06, UTM^-02, UTT^-04, WLX^-05, Y03, YQQH09, Yos02, ZZTS09]. beyond [CLP^-05, CCK01, Ha08, PP08b]. BH [QZL^-04, SAS05]. Bi [LS08a, WL09b, HZ09]. bi-transition [WL09b]. bias [OM04, SY09]. Biased
bicyclic [EBDPM00]. bicyclo [BE07, BPC01]. bifurcation [CPLF02]. bilayer [CEP07, HNL08, MCR08]. bilayers [JM07b, RG08]. bimetallic [WCS09]. bimolecular [ML00]. binary [Kle02, Kle03, LCSZ09].

Binding
[ABA04, AG0+02, BCP03, RGP+07, ABYM08, AM06b, APG05, AVS09, BWE05, BSP06b, DLRZ09, Dra00, ECM+03, FKG+05, GDD+05, GSS04, HT05, HWW07, HWW12, IO08, JMD+02, JZD+09, KFB05, KS08, LW+09, MK02, MHS06, MLL+08, MRS+07, NHH06, NHH06, OYH09, OIF09, PMGL03, RSP03, RGG08, RK05, RUv07, SOOF05, STSF02, SWV+05, TGGP00, VGMM05, WM04, WFF08, Won00, XL02, ZFL01, ZWB09, KEB04].

binodal [MM07]. binuclear [GS04, PLC08]. bio [KH01]. bio-molecules [KH01]. bioactive [BLB09, SD09]. bioactivity [LJZ+07, SJJ+04].

bioinorganic [MSH+06b, SGD06]. bioisosterism [DPM09]. biological [CCK01, CMGDAC+07, GaAcV+07, HMMS09, LTD10, Mac04, TH02, WCK00, YPNE09, vdVG00]. biologically [CSU05, LLL03, RZWS07].

biomarkers [VGDSU08]. biomembrane [WEE01]. biomimetic [FO08].

biomolecular [BHW00, BBM+09, CAC+05, CHB+05, CvG08, FWH+07, JTR05, KAK+09, KYT+08, LSS04, OVM04, WB04a, WB04b, WB05, WL09a, ZFW08]. biomolecule [ABWT09]. biomolecules [ECM+03, Est07, FEVM01, HMD06, KHY00, MMLC05, QSS01, YN+08, YJF06]. bionanosystem [MO09].

biophysical [Mat03]. BiOX [HZ09, Hua09a]. biphenyl [PCMG09].

biradicals [KC01a]. bis [BLN01, CDL06, PYS05]. bis-heteroaromatics [CDL06].

bismacroaromaticity [HWGB01]. bisphosphatase [MRS+07].

bispin-dine [ACM+06]. bits [PM02]. black [MBP09]. Blind [GZM09].

block [ATM+07, ASS+02]. blocked [RBS09]. blockers [HSM04]. blocks [SSB+03]. blood [CRGN07, HSEM06].

Blue [CPDZH08, HCR07, CRO2, MDC08, SRK+00]. blue-shifted [McD08].

Blue-shifting [HRG07]. BLYP [TCT03]. board [ATMK03, KAK+09]. boat [BP09]. bodies [FR98, FS00a]. body [CCK01, FII+07, FBDG06, Ike04, Le03, SM03, TKH07, LR03b].

Bofill [Qua01]. Boltzmann [WB04a, WB05, ABWT09, BHW00, BFF09, BH03, BF04, BP07, GP01, GCD+08, GGT08, Hg05, HBW00, HW01, KHH07, LDG02, NYTH09, PZ04, SAT04, VZM+08, WB04b].

Bond [JG03, MGCA07, May07, SH08, WM12, Bic09, BL06, CMLS05, CPLF02, CPDH08, CJW+09, Cz08, DR09, DGD+05, DMZT08, FH01, FO08, GMN07, GR07, GS07, HG07, HS07a, Hir08, JPCA08, JP09, Klee03, KBLP09, LC07, LZZC09, LS08c, LS05b, MG00, OO04, Pac06, PSC+01, PAS07, PYS05, PV07, Rao00a, RM07, RCJ02a, RD00, SEKS09, Sha07, Sim07, SPT+03, SWZ04, SMZ05, SMW09, ST01, SSW+07, TGM+03, TRu07, VK06, VBGL+00, WHRG08, WJ00, WWXC08, vLBB12].

Bond-based [JG03]. bond-order [LS08c].

bonded [CPDZH08, Gon07, HT03, IO08, LB05, LDL+09, LZF+09, McD08, MH08a, NBTN04a, NBTN04b, NL08, PHFC04, ZH08, vEMK01, vEO1]. bonding
[AM07, AG00, Bac04, Bac05, Bac07, BHTCG07, BM07, BSG07, CWWS07, CQ04, CCK01, EFDQ09, FLK+07, FK07b, Jac09, Kau07, KJP+07, KBL08, Kle02, Kle03, KGD06, LW07, LWO8, LDL+09, PG01, PYCD03, PLC08, RPNJ07, RP04, RS07a, RS07b, SM08a, SG07a, SCP08, Wil01a, WD08, WWS07, XZ04, XK08, Y09, ZW09, ZB07]. bonds

[Bac05, BUMCMRL00, BRS07, CRC+08, DR07, HA04, Mit01, NHH05, O08, PG06, PC05, PC07, SO09, SG06, SJW09, YT04]. Book

[Bic09, Lip00, Sta00, Woo01]. borane

[ZZZ+06]. borate

[HT05]. Born

[LFSB03a, BC06, CF06, DLG00, FOL+04, FC06, GZL02, ILB03, Lab08, LFSB03b, MTE04, MCM04, OCB02, Tot04, XL02, YF06, ZGFL01, ZWZ09]. Born/volume

[Lab08]. borohydride

[QZL+04]. Boron

[JBGK08, LMGR05, LMGR06, LX07, LWLS07, SRS07, ZB07]. Boron-doped

[JBGK08, LWLS07]. boronyls

[LMGR05]. BOSS

[JTR05]. both

[HdMdS05, HdS06, HD06]. bound

[CJPZS08, WC09]. Boundary

[BH03, ABWT09, Ara04, BVW04, BF04, BF07, HH04, KWWH07, QSS01, TK08, WM06]. bovine

[MBC08]. bowls

[LMGR05]. box

[LM03, WM06]. box-counting-based

[LM03]. boxes

[MMP09]. Boyd

[Sta00]. Br

[FHF+01, HZ09, Hua09a, KBL08, Mar03, RB01, STC+08, WLLS04, ZJM+07, ZY01, ZL09b, HYA02, LDC+07, RFSS06, SLL+04b, WLLS05, ZZW+07]. brain

[CRGN07, HMSM06]. BrCl

[WLLS05]. breakage

[SWR06]. breakage/closure

[HR05, Pac06, VHR07b]. breast

[VGD05]. Breit

[Isb03]. bridge

[CFC+08, PAS07]. bridged

[LHP01, SMM+08]. bridges

[KF03]. broadly

[PB05]. broken

[ATH+03, BB08]. bromine

[WyLG+09]. bromine-substituted

[WyLG+09]. BSSE

[GA06, PSC+01, SPDS01, SAM06]. BSSE-corrected

[PSC+01]. BSSE-free

[SAM06]. Buckminsterfullerene

[NRKH02]. buckycatcher

[Won09]. Buff

[KS06]. build

[BMTSC01]. build-up

[BMTSC01]. Building

[BCIB05, BAA07, GKK07, HP05, MABM09, PC00, PFC03, Fau01]. built

[GF05]. bulk

[BACJCT01, BGC+09, EBL+08, JBGK08, LZZC09, LLL03, PB05]. bulk-doping

[JBGK08]. butadiene

[GRO+03, Hir08, WR07]. butanal

[NSB08]. butanes

[WW04]. butyl

[Bac09].

C

[Ano00, BAL+01, BPC01, BS05, Bic09, CTFC08, HK07, mJlZyL+08, KYFW07, KJP+07, KSN01, LJY+08, Mck07a, Mck07b, Owe05, SLL+04b, VBS09, WLL01, WDXS06, WZZ+09, XFF06, YHD+06, ATBL04, Ber03, CPDZ08, CCB04, CS01, CRS03, CTFC08, DGD+05, DRAS04, Ei07, FHF+01, GYD04, GZ07, GB02, HBM06, HYA02, HK07, HA04, IN08, LMR01, LMK01, Mir01, O04, PRSM03, PV07, RD00, RFSS06, SLL+04b, STC+08, TYN05, WLPF05, WDWS06, Wil01b, XDS06a, XWXC08, ZL04, ZW09, ZLD09, ZVRSC08, dRLSM00]. C-PM

[CRSB03]. C12A

[BRDC02]. C12A-p8

[BRDC02]. C96

[ONHN00]. C

[WZZ+09, WD08, XWC09, HL09, PNG08]. cabonyl

[RUPH06]. CaCO

[SCP08]. cage

[CS01, KFD06, WLPF05, WL09b]. cages

[CJS+03, Wan09].
calcium [HSMT04, HLB09, LGB+09, MHJS06]. calcium-induced [LGB+09]. calculate [BACJCT01, CSD04, IS07, Kar01, Kne05, KBLP09, OV03, RSN+02, SFRRS01, WW03, YS00]. calculated [BE06, BE07, GG09, Gra07, LMB07, RM00, Wib04, WM04, ZXY08, KLE03]. calculates [ATMK03]. Calculating [Chu07, CG05, DRMD03, DF04, LN01, MC06, PDC+08, PMM05, RSE07, SYC03, WCK00]. Calculation [BK00, CPML08a, DJ04, KKY01, KRM+02, LSW+01, MT03, MO01, MRS+07, TS05, VM02, VC04, WKY01, ZWPR+04, BP02, BSC+01, BH03, ECA06, FOL+04, FROD08, GKRG08, GLMV09, GADGM08, GGT08, HTKG08, II02, ITN+05, JJK+00, KFNH08, LFK05, MGLO03, NRKH02, Nil09, OCP02, PZWG+04, PRSMV08, RNG03, Rap06, RLER+04a, RKA+09, RRFC+03, SOOF05, STSF02, SM08, SHH07, TZX01b, TZX01a, TLOG00, TRS02, TKN+08, UKN04, UIHN09, WLL+07b, WSM+08, WM01, XOW+00, ZWB09, ZL09b]. Calculations [YH07, Ano01b, ALKH04, Bac09, BP07, BS0B05, BMRDB01, Blo04, BMB07, BMRF01, BWI+02, CLP09, CMJ08, CN03, CRS05, Chi03, CS03, CMA+08, DB07, DPDG05, DSS03, DMJV05, DWC+03, EK0+01, EBL+08, EL09, FKG08, FL08, FMSA06, FR06, FO04, GJL+08, GBDP05, GM04, GWM+00, GBO7, GPS06, HHHB00, HLLN06, HYA02, HSM06, HFL06, HKHN08, HT03, HWGB01, HZ09, Hua09a, Hua09b, IL09, IGL07, IPN06, IN07, JCA+02, JBGK08, JCHS07, KGL07, KWHH07, KRLD09, KTM02, KOB03, KBLP09, KSO2b, KSK04, LL0A01a, LL0A01b, LL0A1c, LL0A1d, LL0A03, LFSB03b, LDC+07, LH09, LWH06, LC06, LKW04, LZF+09, LS05b, LDG02, LM099, MMLC05, Maz08, MBL+00, MA05, MLCD01, MLJ03, MS01, Mui05, NYK+09, NTH09, NSU+02, OBBS05, OYH05, OS06, ORH+02, OOS09, OK0E+02, PB06, PML03, PV03]. calculations [PBZ00, PRSMB01, PSS+04, PSMB05, RSP03, RMP01, RP02, RRCA08, ROC00, RWBH09, RS05, RR0S07, RJ0L06, SBI08, SSB+03, SCS07, SGB+09a, SHM04, Sha02, SSL02, SNO6, SFRRS01, SM09, SG01, TK08, TY03, UK0S01, UTM+02, VPK+08, VZ0V06, Van02b, VE09, VIP+06, WL02, WTKM06, Wh08, WC04, WIF08, WR07, WFR08, WH+07, WJ00, XL08, YTH01, YK08, YSA+03, ZS08, ZXYF09, ZM03, vGGB00, vdVGM00, LFSB03a]. Calibration [OK0+02, LL0L09]. calix [RRZ08]. camphor [AST06]. Can [DSB+02, DDBP09, LC07, MSH+06b, PB06, SB08, STSF02, WS07, IGL07, Mck07a, WC0F4]. cancer [VGD008]. Candida [RGP+07]. candidate [SF07]. canonical [BP02, EMP07, ITN+05, IS07, KM00, Kni00]. CAOs [PS03]. capabilities [GCD04]. capped [CZ05]. caps [ZC03]. capsid [KCL06]. captopril [AGO+02, APG05]. capture [YX+07]. Car [JP09, Sch04]. carpabapen [BB0S06]. carbaole [YFR05]. carbenes [HA04]. Carbohydrate [KBN02]. carbohydrates [ACLD03, HR08, KDS02, LR03a, LCA03, LCA03, LCOA03, LIOA03, LH05, MW00, St05, KYT+08]. Carbon [KK08c, LMG05, BS0B05, BG07, CZ05, CDPL09, DWS+09, GKK07, HT05, KT08, KLS02, KKL01b, LMK01, MMRVH07, PAS07, wQZsLyZ02, SRS07,
Wan09, WSC09, XWL+09, ZKZ+07, ZWY+09, ZZvRSC08. carbon-
[ZWY+09]. carbon-centered [WSC09]. carbon-rich [CZ05]. carbonate
[vDSSvA04]. Carboxyl
[RD00, DLr+08, LL00, LLA01a, LLA01b, LLA01c, LLA01d, LLA03].
carboxyls [BRV+07, LMRG05, PLC08]. carboplatin [WM01]. carboranes
[JRJ01, OSA06]. carboxybenzoxazole [UTH+03]. carboxylates
[CJPZS08]. CarC [BBSS06]. carcinogenic [EL06]. carcinogenicity [VS08].
Carlo [AGSFAL05, AGSFA+05, BR03, BHG03, Der00, FCK+08, FKFG08,
HH07, HMD06, IM06, IKYM09, KL02, KM07, KKC05, LML+00, LZA02,
LR03, MH09, Nak02, NA06, NCO+05, OM04, SKGS00, SCS07, SBJ08,
SM08b, SSW06, TS05, XGK+05, ZCS04]. Carlo-with-Minimization
[NCO+05]. carma [Gly06]. carrying [Tor02]. Cartesian [LPK07, PHY+05].
CAS [PRSMM03, MBM07, JHPRS+05, PRSMM02]. CAS-SCF
[JHPRS+05]. CAS-SDCI [BBM07, PRSMM02]. case [AB00, AS08,
BU07, LL08b, MS04, NT00, RW01, PFB09, SPT+03, WC08, ZAT07].
catalyzed [AST06, BTP09, GVATG03, GLH+08, HSWW00, MCK05, OYO1,
PHK07, RR02, SIE01, TH02, TGLL07, WCW08, WCH09, ZWS+09].
catastrophe [PA05]. cathepsin [ZWB09]. cation [DSB+02, Don08, LB09,
OO04, PV07, QZL+04, SLRC01, VL00, WLZ+07, WSM+08, Wou00, ZL05].
cation-water [DSB+02]. Cationic [JRJ01, TBG00]. cations
[ALC08, GB09, GS04, GLW07, HIA03, Hol05, NSB08, RRS06, SZT08,
WWT08, ZWY+09]. caused [LPK07, TT08]. cavities
[BCIB05, BHH+09, IME02]. cavity [RRZ08, ZFL+05]. C — [CJW+09].
CB [FHF+01]. CBS [Lu09]. cc [Wib04, GYM07]. cc-pVTZ [WD04].
CCH [ZKZ+07, ZKZ+07]. CCl [ZLS06a, FHF+01, WDZS07]. cclib
[OTL08]. CCN [JW06]. CCSD [BBI+09, Lu09, PFJ+03, PV03]. C
[GPS06, XB08, BMRF01, BBI+09]. CD38 [UNHYT06]. CODECKER
[WBVS03]. Ce [SNM+06]. Ceccarelli [An06]. cell
[Got07, KV+09, KS06c, LEV+09]. cell-based [Got07]. cells [CCC09].
cellular [XWC09]. CeN [VP08]. centauric [PA05]. center [BR07, GGA00,
IN01, Lai07, MGGM07a, MGGM07b, NR04, OON01, SG09, TBG00].
centered [CCK01, SSB+03, TBSM09, WSC09]. centers [GYMM07, JKL08].
central [CGMPT+08, CM09]. CeO [CCJ09]. ceramic [HZX04]. cesium
[HD06]. CF [mJZL07, YLW09, LDC+07, gThDjL+01, UTM+02,
UTT+04, WLL+07b, YLYL09]. CFCl [mJZL07]. CFF91
[TTB01a]. CFMC [NCO+05]. CH
[CPJ00, GBDP05, HTN03, IN08, mJZL+08, LW04a, LDT+02b, MGLL03].
chain

chains

chair

chalcogenides

challenge

challenging

chameleonic

Change

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channel

channels

chaos

character

characteristic

characteristics

characterize

characterizing

charge-based

charge-density

charge-scaling

charge-transfer

charged

CHBr

CHCl

CHCR35CHF2

Chibe

Chebyshev

CHEC

CHEC

chem }

Chemical

chemical reaction

chemical species

chemical structure

Chemistry

ChemSpider

ChemViews

charm}

CHARMM

CHARMM-GUI

charge transfer

charge density

charge-based

charge-scaling

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SC01, SS05, SHH07, SFRS01, SCP08, TLOG00, True07, TT02, UNM+01, VBS09, VBGL+00, VKCK09, WS05a, WFHP01, WHP02, WWS07, WZXY07, XYN+06, ZB07, ZMH+09, HP05]. chemically [AVS09, Bud07, SB01, PP08b].

chemicals [CMGDAC+07], chemisorption [KKJH08]. Chemist [SH08, Bac09, Gan09]. Chemistries [DK01, EA08]. Chemistry [Ano05b, Ano06a, Ano06b, Ano06c, GBL+05, vRS98, WB04a, WWCP+05, WHE01, You11, tVBB+01, APG05, BWMO9, BT00, BMRDB01, BS06, BSJ01, CMaGL+04, CFS+08, CMGDAC+07, CMCB08, CMa+08, DBM03, FJP07, FKRE08, GDPCPU07, GDPP08, GdSuM+07, GdAcV+07, KSB+02, KBA+04, KJVW08, KVLY03, KCO1a, LX07, MGCA07, MR09, MBP09, MRRVH07, MFPO0, Nye07, OTL08, SH07, Sha07, SBB02, SGG06, TPH07, YS02, Ano01c, Ano04b, LB99, Lip00, Sta00].

chemistry-based [SBB02].

chemists [Pra01]. Chemometric [HPL03, MRS09]. chemometrics [BLF02]. Chemotaxis [FC06]. Chemotaxis [FC06]. CHEF [UTT+04]. CHFOCHF [YLWL09]. Chichester [Lip00]. Chief [Lip00]. CHIMERA [NCU+02, PGH+04]. Chiral [ZPL07, CGMPT+08, Sza08, ZOJ+06]. chirality [CGMPT+08, PDC+08].

chlorinated [DA01, WDZS07]. chlorine [mJlZsLyL07, mJlZyL+08, WLL07a, XLL+02]. chloro [JKM08]. chloroform [CCK01]. chloroform/water [CCK01]. chlorophylls [LKT04]. Choice [Duk01]. Cholesky [SKD008]. cholesteric [HHBH00]. chromium [RRS06]. chromophore [DHM+03, HFS+07, KHF+09, XZ05]. Chun [Ano06c]. CI [Ano01b, DHE+03, HFS+07, HKHN08, IK00, dSVA+09]. Cieplak [Ano06c].

Circular [AB08, MM00, HKHN08]. cis [DMN05, GRO+03]. cis-diammineplatinum [DMN05]. cisplatin [BZL05, RP04, WM01]. CL [FK5+09, CRC+08, DMN05, GZ07, Han01, HYA02, HTN03, HZ09, Hua09a, mJLZyL+08, KBL08, LF02, Mar03, RB01, STC+08, WLL04, WDZS07, XFF06, ZY01, ZL09b, BS03, HLLS05, mJLZsLyL07, RFSS06, SLL+04a, WLLS05, YLW+08, YLWL09, ZWL+05]. class [CRK08, EBD+01, LL07, VIP+06, YNW05, hYDN+08, Car02, PCS04]. classes [CLF+09, KH06, QLHL09, XSHC06, XLC08, WC09].

Classic [SRE08]. Classical [ATBL04, COL+06, DK01, LLM09, MA05, Nil09, RP07a, STH02, Zho06]. classification [GDPCPU07, gGWH01]. classifier [CLF+09]. clathrate [EM03a]. clay [ATH+03, DJT08]. cleavage [CLXC02, NLL+09]. cleavages [XWXC08]. cleft [SPT+03]. closed [DSB+02]. closed-shell [DSB+02]. close [JRJ01]. closure [CSJ04, DLSVY00, Mak08, SW06]. Cluster [AHG09, Crl04, BR04, BP01, BGJO1a, BWI+02, IN08, JBGK08, KKJH08, KSTC01, LMJ02, LWX07, LYS08, Mck07a, MS01, Mor02, NK06, PSF+08, SS07, VDM06, WKYU01, Whe08, WXJ+08]. cluster-continuum [WJX+08]. cluster/adsorbate [BW1+02]. clustered [FPN+05]. clustering [CCWH02, FKZ09, LZ05a, LOL+08, RLA01, ZS04]. clusters [BP00, BACJCT01, CGG06, CAG07, DSB+02, GBBH09, HX08, HYR06, JHMB+09, JHMB+11, JG03, KGL07, KDG+09, KZW+05, LML+00].
LWLS07, LJS05, Mck07a, Mck07b, NB04, OSHS03, OS08, PBZ00, Pul05, QB05, SCC04, SYC08, SW06, WLL01, WZZ+09, WCS09, XZ04, YCS07, ZLJS03, ZXL+04, ZWC+09, ZXY03, ZGXX06, ZX09, ZB07, Est07]. CM1 [UBDPJ04]. CM3 [UBDPJ04]. CN [LW04a, TJM+03, TYN05]. CO [GD06, PLC08, RD00, TJM+03, VS02, KT08, ABYM08, DLD+02, FLK+07, PBZ00, SS05, PLC08]. co-ligation [KT08]. CoA [LLL+08]. coagulation [PDP02]. Coarse [CA07a, EBAN07, VTT+08, CP09, DR07, DJB02, HXLS09, MBC08, PSHP08, SB08, WWL+09]. Coarse-grained [VTT+08, CP09, DJB02, HXLS09, MBC08, SB08, WWL+09]. Coarse-graining [CA07a, EBAN07]. coastline [UTH+03]. cobalamins [KPZK06]. cobalt [LMIF06]. cocaine [ZDS+05]. cocrystals [CWV+05]. code [BDW00, FROD08, GBL+05, GJK+06, GY08, PZWG04]. codification [CGMPT+08]. coding [LCSZ09]. coecient [CSB+03, YSJ09]. coecients [CCK01, DA01, GS09, Gol09, LZZC09, Whe08]. coenzyme [WC08]. cofactor [Mck07a, Mck07b]. cofactors [Ano06b, CPM03]. cohesive [VP08]. collections [CDD+02]. Collective [CCSJ00, HSWN01, LV08, SWR06]. collide [CKF01]. collinear [Van02b]. collision [VW00, VW04, TYN05]. Collisions [Pan07]. co-localised [CJDK09]. collocation [CRK08]. collocation-based [CRK08]. colony [CLZ+09, CLZX09]. comb [LAEL01]. comb-like [LAEL01]. Combination [MH08b, DLD+02, GHH07, HSWN01, KKS04, dSR08]. combinations [ZOJ+06]. combinatorial [AL01, GD09]. Combined [CYM02, GWM08, KBLP09, RG02, ZKZ+07, BAL+01, BCN+07, BME05, COS01, DPT03, Der09, FSFK05, KH01, KM00, LMCD09, MC06, Oos09, TCR+02, VMF+03, WX09, XLZ08]. Combining [MBC08, SS00, HTKG08, KN04, LLZL09, ZM09, KK08b, LEK07]. comblike [LZA02, ZALMG03]. CoMFA [JFG04]. Comment [CPML08b, JW12, Kne05, Qua01, Van08, Bof01, CSD05, WM12, vLBBR12]. Comments [MBP09]. Common [ZAT07]. commonly [ESP04, SCF+09]. Comp [HNWF12, Kne05]. compact [Kri09a]. comparably [PB02]. Comparative [CCP04, GHLK+02, LS02, SBJ08, SCF+09, Sto05, VMA03, CMD+04, FC06, FO08, GM01, HLMR06, JFG04, KS01b, LPK07, McDo08, PHKG07, PMM05, TBG00, WC09, EBL+08, JHZ09]. compared [IO08, JCHS07]. Comparing [JCL05]. Comparison [AEE+03, Bou00, CV09, DB07, DLG00, GGLR00, Kr03, SL06, SDL07, TCR+02, WMGK07, WMW03, YLL+09, ZL09, AE06, BL05, FOL+04, FDSA00, GDPCP07, Gra07, HRKB03, JARM02, LC07, LOL+08, LZF+09, MZ05, MS00, MST+08, MC06, PK04, PS03, RDM+08, SBLK01, SB05, SSB07, WB04b, WB05, BRDC02, CCT+03, COL+06, LKT04, NCO+05, ONH00, PSF+08, SPDS01, SL04, SKK+07, WMW04, YKK09, ZGFL01, ZOJ+06]. Comparisons [GPK05]. COMPASS [MSR04]. compatible [BSDM04, KH06]. competing [HA04]. competitive [FG03].
complementarity [EKB02b]. Complete [BT00, MLL+08b, Pog03, PRT+07, PRT+08, MC06, Var09, WMRW+01]. completeness [AHK02, MV06]. completeness-optimized [MV06].

Complex [DFGB09, AS06, Bac09, BRS00, BRS01, GC04, HDF+07, HDO+02, HMK02, IV04, IsSV06, Ish04, JLFH03, Kle02, KVS+06, LB05, LDL+09, MM03, MCF05, MY08b, MY08a, NHN06, Pac06, ZWB09].

complexation [AGI+07, HT05, LMMW04, SRK+00, SLRC01]. complexed [Pin03, SDM02, WCF04]. Complexes [APG05, AB00, Ano06a, ACM+06, BTP09, BR04, BL06, BM00, BGC+09, BZL05, CG03, CBC+08, CSB08, CBH+03, DPT03, DF04, FRS05, FO08, FRLN09, FKS+09, GTC06, GL04b, GM01, GSPS06, GP05, Gni04, GZW09, GWL07, HLLN06, HRG07, IO08, IGO7, JMD+02, JD09, JCHS07, KT08, KRM+02, KJP+07, LL00, LHH+06, L02, LMGR06, LLS03, LMMW04, LWZ09, LZF+09, LS05b, Mas04, McD08, MHJS06, MSBS01, MLL+08b, NHN06, NR04, NMAT01, PGG06, QTdG+08, RPNJ07, RMP01, RRFC+03, SG07a, SCF+09, SBH02, ST06, SVV+08, TGGP+00, UM03, VS02, VMA03, VL00, WB07, WWT08, Won09, ZY01, ZBS03, ZZY+09, ZTS09, dBV01].

complexes* [GK09]. complexity [BT00, PK05, XSHC06]. Component [KBA+04, CCT+03, GSPS06, JMD+02, PVdJB00, PV03, SH02, SM08b, Van02b, Wan03, YS01, ZBS03, ZYY+09, ZTS09, dBV01]. complexed [Pin03, SDM02, WCF04]. Complexes [APG05, AB00, Ano06a, ACM+06, BTP09, BR04, BL06, BM00, BGC+09, BZL05, CG03, CBC+08, CSB08, CBH+03, DPT03, DF04, FRS05, FO08, FRLN09, FKS+09, GTC06, GL04b, GM01, GSPS06, GP05, Gni04, GZW09, GWL07, HLLN06, HRG07, IO08, IGO7, JMD+02, JD09, JCHS07, KT08, KRM+02, KJP+07, LL00, LHH+06, L02, LMGR06, LLS03, LMMW04, LWZ09, LZF+09, LS05b, Mas04, McD08, MHJS06, MSBS01, MLL+08b, NHN06, NR04, NMAT01, PGG06, QTdG+08, RPNJ07, RMP01, RRFC+03, SG07a, SCF+09, SBH02, ST06, SVV+08, TGGP+00, UM03, VS02, VMA03, VL00, WB07, WWT08, Won09, ZY01, ZBS03, ZZY+09, ZTS09, dBV01].

Component [KBA+04, CCT+03, GSPS06, JMD+02, PVdJB00, PV03, SH02, SM08b, Van02b, WG02]. Component-based [KBA+04]. Components [KJVV08, Car02, LL07, TGGP+00]. composition [HM06, KWHH07, LL07, PAS08, XSHC06, XLC08]. Compound [CN05, BR07, HBM06, RD00, ZK05]. compounds [ACLD03, BB08, BLO+02, CYM02, DA01, EBDPM00, EDAJ04, EBD+01, FJ08, FROD08, FO04, Go09, Gor01, JLFH03, KFD06, LLA01a, LLA01b, LLA01c, LLA01d, LLA03, LD05a, LWK08, LT+07, LW06, LCDA03, LC03, LCO3, LJZ+07, LLM09, MD04, NBTN04a, PZWG+04, PYCD03, POJ01, RUPH06, SJJ+04, ST01, TMBM09, YCW+09, YSA+03]. Comprehensive [LF02, ZL09b, ZB07, DL+08, JFPS+00, SL05].

compression [BG07, MBWP03]. comprising [Rud05b, Rud05c]. Comput [Bo01, Qua01, Van08]. Computation [Bo01, Qua01, Van08]. Computationally [KM00, KFZ03]. Computations
compute [BDW00, RKA+09]. computed [PFJ+03, PK05, TDH06].
computer [HFSD03, H605, NK01, PPXP01, PHJ+08, TRS02, UIHN09, VB07, VKCK09, YNZ+08, Zer08]. Computing [HHW+03, WL00, BHH+09, DGRH02, DP04, DK01, GLD08, HHS+05, KFB05, LM03, MA09, ZP03].
CONAN [SSHT03]. concave [Won09]. concentration [GGT08]. concept [LSY02, Rao00b, Rud05a]. Conceptual [VB09]. Concerning [FG03, Bo03]. concerted [LFS+07, Mck07b, NSB08, LLKC06]. condensed [CLP09, DG08, DWC+03, FM00, GLMV09, Mor02, SDvG01, ZSK07]. condensed-phase [DWC+03]. condition [SK08]. conditions [BVW04, CEP07, HH04, WL00, BHH+09, DGHR02, DP04, Mak08, MH08b, MA05, MGJAR00, NKS02, OML+00, OGH05, PRT+07, RIO+08, SPL+02, SWBM08, SHBD05, SD09, SSBE06, WCK00, YXL+09, ZAR07, CG03, HJCP01, JP07+00]. Conformations [NHH05, CLWL09, CI05, yChn08, DBM03, ENM+04, FW+07, GBB07, GB04, HD0+02, HP05, LZXK04, MW00, OFB08, OKH+02, PC00, PFC03, RAO09, RP09, TLK07].
connectivity [EDAJ04, Pog06]. conquer [AKN07, ML03, vdVGDM00]. consensus [GP06, JMD+02, LLL+08, RHL09]. Consequences [RSS09].
considerations [GRCD01, PB05]. Consistent [RP02, BWA+02, ECM+03, KKG08a, KBN02, NUH02, SMD02, VTT+08, WM04, XL02]. Constant [MCM04, DMR03, Sch00, Vas02, WLL05, WLL+07b]. constants [Chn07, FW06, GBB07a, GBB07b, HFWN01, JHZ09, Kch03, MML05, MGL03, MLD04, PJPJdPRM07, RR+03, SLL+04b, SFRS01, TLOG00, WDX+02, WZXY07, ZXY08]. constrained [COS01, EC06, LFKL00, MM00]. Constraining [AM09, HSW00]. constraint [BL09, FS09, KVGH01, YXC+07]. constraints [BVW04, Bud07, BRS00, BRS01, ECA06, Pen06, PB07, VMF+03].
constructed [Gri06, YCS07]. Constructing [ZBS03]. construction [HH04, RSN+02, TYO+02, UIHN09]. contact [ENM+04]. contained [LH02, SH07]. containing [BS06, FLOD07, FPN+05, JPF+00, LKJ+04, LWW+06, LFR07, LLVM09, MSH+06b, PPC03, RRZA08, SL09, STC+08, WL04, Wil01b]. contemporary [CFS+08]. content [CLC03]. context [KMH02, KBT03, OCP02]. contexts [Sim07]. Continuous [FZL+06, LF04, LFZS04, ZFL+05, HHHS01, SM08b, PDC+08]. Continuum [FCP+04b, MGL03, ABWT09, BCIB05, CFR08, COL01, CCT+03, COL+06, FKL+06, FEVM01, FBL08, GS02, GWS+02, HC08, HS01, HHP04, KKS04, LRI+02, LJ04, MWL+08, Pom04, RSP03, Sch00, STSF02, TJE03, VP09, WJX+08, YCBM00, ZFW08]. continuum-solvation [Sch00]. contours [YGZZ05]. contracted [GS09]. contraction [CGSdST06]. contribution [BCIB05, CR09a, DBS07, KC01a, LKA01, PWHF+03, PWHF+04, PMPGP05, RI07]. contributions [CBC+08, CR08, CSB+03, COL+06, GPK05, HIM07, MGL03, RM07, SVW+05]. Control [Kar06, DB06, LR06, MN02, RS05]. conventional [WMW03, WMW04]. Convergence [KGN07, LST08, GG09, LTV08, LJ04, Mas04, Rud05a, Rud05b, Rud05c]. convergent [PAS08, Zho06]. Converging [GC04, KF02b]. conversion [CC09, CFDO4, PRH+05, RR05]. converting [RM00]. Cool [BHG03]. cooperation [ATMK03]. cooperative [HLB09, RRCA08]. coordinate [BGC+09, HDBD04, Ish02, KTA03, LN01, RWBH09]. coordinated [GWL07, Sha02, SBH02]. Coordinates [EA06, Din00, EC06, GKK07, KSU03, LPK07, NKS02, QCK01, QCK02, TNS00]. coordinating [JRJ01]. Coordination [KZRO03, Gor01, HXD08, SFR07, TBG00]. coordinations [DSB+02]. Cope [PA05]. copolymer [CHA+07]. copolymers [YFR05]. copper [CR02, DBS07, FNP+06, PMGL03, PBZ00, PS03, ZWC+09, ACM+06]. corannulene [Won09]. core [ATM+07, CM09, FR06, HX08, HYR06, HIJP01, ION07, LF05, LK03, LK04, NTH09, ON07, Pog03, TJM+03, TLKT00, TJE03, TKN+08, YCS07]. core-excitation [ON07]. core-excited-state [TKN+08]. Cornell [RKH03]. Coronavirus [LZX06]. corrected [NTH09, PSC+01]. Correction [Duk01, CFC+08, GA106, Gri06, HK08c, HK08d, IK08, LBT07, MGLD00, MUE01, QCK01, QCK02, SPDS01, STSF02, TKH03, WX09]. corrections [BF07, Gri04, KSS08, WB07]. correctly [LF04]. corrector [Kol04]. correlate [Kle03]. Correlated [GBB07, BWW+08, BLT03, DBM03, GPSP06, KMA+07, PFBO5, TBG00, WM03, WMW04]. correlating [NSO+07, SNM+06]. Correlation [LRWG03, TDH06, AAP00, AGI+07, AS00, BL00, CKT+08, EL09, FDM00, GKT04, HNO2, HR08, Hir08, IKN08, JJK+00, JSH07, KGN07, KK08a, KC01b, LMJ02, Mat03, PJPJdPRM07, PNC+08, SRE08, TKH07, WMW03, WL04, YH09, dSGCG00, WMW04]. correlations [DR09, HHW+03]. Correspondence [RLRE01]. corrphycene
[NyHN06]. **COSMO** [EK06, ELK⁺09, KEH⁺02]. **COSMO-RS** [EK06, ELK⁺09, KEH⁺02]. **COSMOS90** [SS07]. **counterions** [JD09]. **counterpoise** [GA06]. **counting** [HYT05, LM03]. **Coupled** [BSP06b, MO01, CXZ⁺09, DOSG06, IN08, KSTC01, LMJ02, LYS08, PSF⁺08, SSB07, WKYU01, Whe08, XWC09, SMAV00]. **coupled-cluster** [IN08, KSTC01, Whe08]. **couplings** [BPC01, NR04, TP01b]. **CoV** [LZ05b]. **Covalent** [BSG07, BMTFR08, PML03, RS07a, RS07b]. **covalently** [PHFC04]. **coverage** [SURG06]. **covering** [RKH03]. **COX** [WC09]. **COX-1** [WC09]. **COX-2** [WC09]. **CP** [ZKZ⁺07]. **CPHF** [ASWG07]. **Cr** [KPR04, Kri08]. **Crehuet** [Bof01, Qua01]. **criteria** [Kle03]. **criterion** [ALTB06, GLD08, PSDM00]. **Critical** [GT03, BMLV04, BLN01, BAA⁺07, CRC⁺08, CKMC04, FMP08, LFR⁺04, MP03b]. **cross** [GAN09, MY08b, MY08a]. **crosscorrelation** [HWDB03]. **crossed** [BAL⁺01]. **crossing** [LI07]. **crossings** [LSG06]. **crossover** [KRLD09]. **cryogenic** [HN02]. **cryostat** [WWT08]. **Crystal** [KOFF09, Van02a, DPT03, EL09, HN02, KP05, TD08, VVBV02, vDSVA04, vEMK01, vE01, DRMD03, FROD08, PZWG⁺04]. **crystalline** [AS00, CADW03, JB04, PZWG⁺04, Wil01a, ZLD09]. **crystallographic** [RON02]. **crystals** [BCF⁺09, CC07, FA01a, GAdGM08, GBJ03, PMC⁺08, RD06, WMS06, Wil01b]. Cs [GWL07, GLRL02]. **CSA** [NCO⁺05]. **CSOV** [GPS06, PMPG05]. **Cu** [BTP09, GPS06, Sha02, HS08, NK06, TDK07, WCS09, ZTP⁺08]. **CuN** [ZX08]. **cuprates** [MD04]. **Current** [NYTH09, CDPL09, Vis02]. **curvature** [TRS02]. **curved** [ABWT09]. **curves** [BBI⁺09, MM07, SSS⁺09, ZLY07]. **Customized** [BDW00]. **cut** [BME05]. **cutoff** [GGT08, KLM⁺09]. **CuX** [KBL08]. **cyanines** [BG00]. **cyano** [PA05]. **cyanoacetylene** [YDWS06]. **cyanobiphenyl** [CC07]. **cyanoboranes** [WC08]. **cyanomethyldiyne** [WDS06]. **cycle** [ZAT07]. **Cyclic** [KJP⁺07, BGJ01a, CLA⁺00, FKM⁺06, FKM⁺07, JBKG08, LXL07, OYK⁺09, VVS07, WOC⁺03]. **cyclic-AMP** [FKM⁺06, FKM⁺07]. **cyclization** [PWFS01]. **cyclizations** [SGS03]. **cyclo** [TDK07]. **cyclo-Cu** [TDK07]. **cycloalkanes** [SBE06]. **cyclobutane** [QZZZ03]. **cyclobutene** [SRE08]. **cyclohexane** [MT03, RP09]. **Cycloketones** [LLA01b]. **cyclononane** [SBE06]. **cyclononatriene** [ZSE08]. **cyclooctatetraene** [CPFL02]. **cyclopentadienyl** [ML00]. **cyclopentene** [SURG06]. **cyclopeptidic** [FL07]. **cycloreversion** [QZZZ03]. **CYP2A6** [VB09]. **cysteine** [CN05, MOP⁺07, PMM06]. **cysteine-6** [PMM06]. **cysteines** [CFR06]. **cytochrome** [AT06, ATBLS04, HBM06, JKL08, LCC09, OYH05, OON01, ZAT07, BS06]. **cytosine** [KMMMS04, MDA08, MHS05, MI08a, SBI08, SG07a, SC01].
cytosine- [MHS05]. cytosine-5-acetic [MH08a]. CZ [CRC+08].

D [IS03, PF06, SHBD05, AGO+02, BAH+02, CPC+00, DDBP09, DMC05, FR0D08, GDPCPU07, GdSuM+07, GdAcV+07, HP05, LW04b, LZX06, LW06, MP03b, OYK+09, RSSKB03, RGP+07, SFC04, YNW05, hYDN+08, ZTS09, vDSSvA04, TGLL07]. D- [AGO+02]. D-arabinonate [RGP+07]. D-arabinonohydroxamate [RGP+07]. D-Epitope-Explorer [SHBD05]. D-erythronic [vDSSvA04]. D-galactose [RSSKB03]. D-QSAR [DMC05]. D-RNA-coupling [GdAcV+07]. D/ [PF06]. D180 [NYK+09]. d2 cluster [CCWH02]. damage [FPN+05]. dangers [MBP09]. data [ASWG07, BRDC02, BK00, CDD+02, CRGN07, FOK+04, FM00, HHJ03, HSWN01, KMH02, KMA+07, LEK07, MBWP03, MMP+07, PFJ+03, PF06, RLA01, RRS07, RRS09, RON02, SY09, SFC04, WG02]. database [DPM09, LFKL00]. databases [BR07, PPXP01]. dative [FH01]. David [Woo01, Ano05b]. day [GR07]. DD [ZLY07]. DD-curves [ZLY07]. Dead [YFS07, Add04, GLD08, KUB07, PSDM00]. Dead-end [YFS07, Add04, GLD08, KUB07, PSDM00]. deaminase [MDA08].

dearomatization [HT05]. debates [Nye07]. decarboxylase [HLC09, LLL+08]. decarboxylation [UTH+03]. decker [RPNJ07]. decomposable [VZM+08]. decomposition [BM07, CBH+03, FKO7a, FPG+06, Hir08, KZY09, KN04, LBG08, ML00, SKDO08, TBSM09, TCR+02, ZZL04]. decompositions [GPS06, PBF07]. decoys [LZ05a, SRCD03]. defect [ZMH+09]. defects [JT08]. Definition [EA06, LFSB03a, LFSB03b]. Definitions [PBF07]. Definitive [dOMSL01]. deformation [GBB04]. deformations [Din00]. deformed [RLER04b].
degenerate [NUH02]. degradation [PCMG09]. degree [CC09, RLER07].
degrees [DHF+05, MZL08]. dehalogenase [NYK+09]. dehydration [TT02]. dehydrogenase [SS05].
dehydrohalogenation [TT02], deletion [SHH07]. delineate [MP03a].
delocalization [BY06, BJO6, FVB08, FS02, Kar06, MMGM07a, MMGM07b, WMW03, WW03, WMW04, Wan09]. deltorphin [OM04, YAÇ+02].
deMon2k [GJK+06]. denatured [GB04]. dendrimeric [SCG04]. densities [GY08, GB03, HSWW00, KCK+08, LMV07, RLR+04, VZVG06, Van02b]. Density [BP01, FG02, Han01, ÍCHS07, KWK+01, KWK+02, MSBS01, QZZZ03, QZL+04, VL00, WCW08, AB00, ABYM08, AEE+03, ASY01, Baco09, BP03, BMLV04, BB08, BAA07, CLP+05, CRC+08, CFK08, CRS05, CR08, CSG08, CAG07, CPML08a, Cu04, CGSiST06, DVP+02, DVRP+03, DF04, ECM+03, FCW06, FZL07, FDM00, FS04, GHLK+02, GLR02, Gri04, Gri06, GBB09, GHHB04, HGBM04, HLS07, HNWF07, HNWF12, HN02, Hir08, Hol05, IIO2, ION07, IN08, IB04, ITN+05, IS07, JNV08, Jac09, JCA+02, JFG04, KG07, KRM+02, KN04, KSS08, Kle03, Kni00, KZW+05, Kri09a, KS01b, LRI+02, Lch06, LV08, LMB08, LMGR05, LLS03, LWH06, LKT04, LF02, LLZL09, LDL+09, LZF+09, MP03a, MV09, MS00, NK06, NTH09, NAT07, OKE+02, PSF+08, RB01, RK04, RLER04b, RDM+08, RR05].
[RZWS07, SH07, SZT08, SPT^+03, SCF^+09]. density
[SLRC01, SSB07, SW06, DBG00, TST^+08, TKN^+08, TKH03, Van02b, VMA03, VBS09, VC04, VCKK09, WR^+06, WB07, WZY04, WMRW^+01, WL02, WCHW09, WM04, WCL05, WZXY07, WM01, XB08, XL02, XPW09, YTH01, YL09, YK08, YYW07, YLL^+09, ZSL04, ZH08, Zho06, ZM03, vGGB00, Haf08, LWK08, MW00, XYN^+06, GM01]. density-functional
[HNWF07, HNWF12, LLS03, LWH06, TST^+08, TKN08, TKH03, Van02b, VMA03, VBS09, VC04, VCKK09, WR^+06, WB07, WZY04, WMRW^+01, WL02, WCHW09, WM04, WCL05, WZXY07, WM01, XB08, XL02, XPW09, YTH01, YL09, YK08, YYW07, YLL^+09, ZSL04, ZH08, Zho06, ZM03, vGGB00, Haf08, LWK08, MW00, XYN^+06, GM01]. density/polarization [YL09]. density-functional [HNWF07, HNWF12, LLS03, LWH06, TST^+08, Haf08].
density/polarization [YL09]. deoxyguanosine [MM02]. deoxyribonucleoside [PFR04b]. deoxyribose [LBG08, SA07].
Dependence [ASS^+02, MGLL03, BRLS08, BRLS12, BL00, KH06, NK06, SR09, TMT^+03, VKCK09, ZP03, ZXY08, DvG00, DPM09, MG06].
dependence [OKH^+02]. dependent [Bac09, CFK08, FCW06, FCP^+04a, Gog08, GS04, HNWF07, HNWF12, HS01, ION07, LDA^+08, LDL^+09, LSW^+01, MML02, MW09, MY08a, NTH09, ONHN00, PSF^+08, TST^+08, Whe08, WC08, YH07, ZH08, ZM03, vGGB00, PM05]. depiction [ZTS09]. deposit [JG03]. deposition [UNM^+01]. deprotonated [Mas04].
Derivation [EBD^+01, JFG04, TT05, TTB01a, EBD^+01, HZ06a, Tor02, Tot04].
derivative [CNN07]. derivatives [BT00, Bor03, BC06, CJK^+02, COMR^+04, DMC05, DOSG06, FL08, GLRL02, IS03, PSF^+08, PA05, QCK01, QCK02, RP09, SPGS08, SGPS09, Sch00, STC^+08, TNS00]. derived [GBJ03, HSWN01, Ish02, KS06, KFNN08, MLJ03, SvdS01, TBSM09, WMS06].
Deriving [RPMP03]. desaturation [BBSS06]. descreening [MTE04]. describe [DDBP09, IDMC09, MSH^+06b, RLDI09, SB09].
describing [CMMaGL^+04, HK08a, HK08b]. Description
[ION07, MHT01, BUMCMRL00, BME05, CLWL09, CHRL09, Grl04, HGB04, SM08a, VMA03]. descriptions [SB08]. descriptor
c[DSD09, RS09, TCSM03, XYN^+06, ZNL07]. descriptors
[AGMPRG^+08, BA07, DA01, EDJ04, HM08, HMM09, Jac09, LXW^+09, MGMM07b, RUPH06, Tio09, TTB09, WNU00]. Design
[AG03, KV00, BS06a, BMTSC01, BLMS08, CRH^+07, CMBC08, DB06, DHW^+07, DHW^+09, GHP03, Ham07, HM06, HLTLP09, HLM05, JGVF05, LFBSK07, LZ05b, LFS^+07, MWE02, NH05, PS09a, SPGS08, SRS07, SH04, STC08, VGGM05, VZM^+08, YFS07, ZSC08, ZL09a]. designed [GT03]. designing [GDV03]. Desirability [CMBC08]. Desirability-based [CMBC08]. desolvation [HMOG07, SWV^+05]. Detailed [PB05, WRBV03].
details [GGB07a]. detecting [BH0+09]. Detection
[WHH^+06, BAL^+01, CMCB08, OYH09]. determinant [GS09].
determinants [BPC03, Bou01]. Determination
[BLT03, CFR06, CR08, DLD^+02, FSS00, Vas02, BL08, BR03, BCNs07, BdPRMAI00, CC09, Chi03, CAGR08, FAR02, GCCVB00, HP05, Mar03, MGLD00, MM07, PC00, PFC03, PAB03, RI07, RTG00, SCF^+09, TBSM09, vDSSvA04].
determinations [YXL^+09]. determine
[DDVD09, KUB07, OO08, RI08, YH06]. determined [OYH05, TDH06].
determining [BY06, DV02, LR06, PHJ+08]. Deterministic [LS05a].
detonation [JWB05]. detoxification [ZWS+09]. developed
[CRS05, KMH02, RG08]. Development
[ATMK03, BGJ01a, HHJ03, IS07, KSB+02, KOML08, KVL+04, LAT05,
LK03, MSR04, MRC03, WWC+04, WWC+05, WS05b, XYN+06, Yan04,
BA08, COS01, CMGDAC+07, KLB03, NG04, BG03, IKYM09, SM08b].
developments [FCP+04b, HS07a, SMD02]. DFT
[BRLS12, ASDP+06, ACM+06, BWP07, BPC01, BP07, BSB05, BM08, BB08,
BE07, BRLS08, BBSS06, BZL05, CMJ08, CCCJ09, CHA+07, CG06, CS03,
CMA+08, DGD+05, Der09, DDP09, ESP04, EKO+01, EBL+08, FO08,
FO04, FKS+09, GCCVB00, GKH05, GPSP06, GKT05, HLLN06, HT05,
HSWW00, HK07, Huo99a, JPF+00, KL02, KL03, KTM02, Kri09a,
KPZK06, LMV07, LKY+04, LDC+07, LWLS07, LS08b, LWZ09, LS05b,
MLM+06, MOP+07, MGG06, MBWP03, PFJ+03, PMPG05, PMM06,
RM00, SBI08, SWBM08, SBL05, SN06, SCG04, SSBE06, SRB06, Tle09,
VS02, VB09, WMGK07, WLX+05, WWT08, WL09b, XXY+05, YS00,
YS08, ZSE08, ZKZ+07, ZWS+02, ZWY+09]. DFT-D [DDBP09].
DFT/MRCI [KTM02]. DFTB [ECM+03].
di- [CU01, GBB07]. di-arsenic [KS05a].
diabetes [PS09a]. Diagonalization [LSAS01, BdPRMAI00, PU09].
diagram [Hir08]. diamide [HHP04]. diaminoguanidine [BI06].
diaminomethylene [TKS+01]. diammineplatinum [DMN05]. diamond
[ECO+01, JBGK08, ZMH+09]. diatomic [OSA06]. diatomic
[ALKH04, FCW06, TLOG00, WWS07]. diatomics [Cul08]. Diatropicity
[CdML06]. diazonium [EL06, EL07]. diborane [wQZsLyZ02].
dibromomethane [LXS08]. dicarboxylic [NHH05]. dication [Bac09].
dichlorides [LHP01]. dichloromethane [RRZA08]. dichroic [MM00].
dichroism [AB08, HKHN08]. didehydrodipyridine [KC01a].
didehydrophenanthroline [KC01a]. Dielectric [HS01, DRMD03, GS03,
HMWC03, HLLN06, LZCO09, MML02, Vas02, ZFW08]. Diels [Hir08].
DIESEL [ME06]. differ [SRK+00]. difference [ALC08, Bie04a, Bie04b,
BF04, PMPG05, PZS04, Rud05a, Rud05b, Rud05c, VZM+08]. differences
[CV09, GG09, OV03, YZ04]. different [ABA+04, BL05, CEP+07,
CMGDAC+07, DS+02, MCF07, MN02, VC04, WM01]. differential [DD08].
differently [HSF08]. diffraction [HH03, dGWH01]. Diffuse [GS07].
Diffusion [VV04, BM09, Bie04a, CCCJ09, Rud05a, VW00, PK04].
difluoroethane [CUS00]. dihaloethanes [WFR08]. dihedral
[FKZ09, HK08c, OFIK09, YL06]. dihydro [WJX+08]. dihydrodilute
[PCM09]. dihydroxyethylene [GGLR00]. dihydrogen [Mck07b].
Dihydroxy phospholipase [CDL06]. dihydroxy pyridine [HSM04].
dihydroxy pyridine [YXZ+04]. diimino benzosemiquinonate [Bac09].
diron [BB08]. diketiminate [GTC06]. diketonate [RMP01]. dilute
[HRR05, Kri09b, XZ04]. dilution [DA01]. dimension [TSMNG01].
dimensional [BP01, Bie04a, CVR08, DHW+08, LAR+03, LR06, MP03a,
MVLT06, RSS09, SHBD05, Wan09]. dimensionality [CDGS09].
dimensions [AHK02]. dimer [CWY09, GYCY04, Kr03, LZJ03, MMPK01, McD03, NK01, RRCA08, SB08, SG07b, YTH01, ZGXX06]. dimerization [HK07, JJK+00, WXX08]. dimers [BBI+09, FKRE08, GYMN07, LMGO+09, NL08, OKE+02, Owe05, RB01, VC04, WXK08, ZOJ+06]. dimethoxyethane [LCGA03]. dimethyl [GGGLL05, GWM+00, WLL+03, WJX+08].

dimethyl-2-iodobenzoylphosphonate [GWM+00]. dimethylacetylene [MTB09]. dimethylallene [ZPL07]. dimethylamino [ZH08].
dimethylcarbamate [KKH+07]. dimethylhydrazine [Lu09]. dinitrogen [Ano06a, ST06]. dinuclear [SMM+08, SDM02]. dipoles [LFR07].
diol [Kle02, Kle03]. diol-water [Kle02]. diols [Kle02, Kle03].
dioxygen [BLO+02, SSW+07]. dipalmitoyl [CEP07]. dipeptide [BISB02, ECA06, HLMR06, JW06, KK09, LRI+02, LL07, PFJ+03, Qua07, WD04, YXL+09].
dipeptides [LSW+01, TTB01b, YXL+09]. diphsophates [PFR04b]. dipolar [RI08, San01]. dipole [DVP+02, EDW07, HN02, HK08a, HK08d, HK08b, KFZ03, MLA00]. dipole-quadrupole [HK08a, HK08b]. Dirac [HDBD04, PVdJB00, TW03, Vis02].

direct [CBS+03, CAG07, JHH01, LW04a, TY03, WLLS04, WDX+02, YLZ08].
direct-particle-deletion [SHH07]. directly [SFRS01]. disaccharide [FKJ+01]. disaccharides [SRB02]. DISCO [ZBS03]. DISCOtech [JFG04].
discover [LHJ+06]. discovery [HS07b, KV00]. discrete [DXW08, MGLO03, QLHL09, YL06, ZBS03]. discretization [Bie04a, Bie04b, RP07b]. discriminant [ZHH09]. discriminants [FTLV01].
discriminating [yCkHmY08]. Discrimination [LDTS07, ZPL07].
discriminative [WHH+06]. discussion [CDGS09]. disilenes [TKS+01].
dismutase [PMM06]. dismutases [RJLR06]. Dispersion [COL+06, RDM+08, CLZX09, GYMN07, Gri06, JCHS07, KSS08, Lab08, Wh08].
dispensive [BCF+09]. dissimilarity [hYDN+08]. dissipative [YCXY03].
dissociation [CJW+09, KWK+01, KWK+02, LS05b, TJM+03, WZZ+09].
dissociative [ABY08, KKJ08]. dissolution [SBG09b]. distal [IGNH03].

distance [MML02, RSS09, Ano05b, BL00, Cri04, IZA06, KwGH01, KH06, LI07, LH09, PYEA03, Sha05]. distance-dependence [BL00].
distance-limited [Ano05b, Sha05]. distances [Var09]. Distorted [KS01b].
distortion [LM009]. distributed [ASW07, DGH02, FOK+04, IS07, KMA+07, SKK+07, TYO+02, ZP03]. distribution [ACM+06, BBP09, CFS03, CV09, CMGDAC+07, JVV09, KS01a, KS02a, LBT07, MZ05, MLG04, PP06b, SK09].
distributions [AEE+03, BSP06b, Ch03, HLS07, LV08, MFB04, RLER05]. disulfide [DWS+09, KF03, wQZsLyZ02].
dithiapentacyclohexane [FD03]. dithiane [FD03]. divalent [GS04]. diverse [AGMPRG+08, AVS09].
diversity [SMM+08, SDM02].
divide [AKN07, MLJ03]. divide-and-conquer [AKN07, MLJ03]. dizincocene [GXK09]. DL POLY [KSY+00]. DMPC [HNL08]. DMS [RAGLL09a, RAGLL09b]. DMS-OH [RAGLL09a]. DMSO [RAGLL09a, RAGLL09b]. DNA [AB08, AZM03, BCP03, DLW06, DLWV07, EL06, EL07, FPN+05, FKM+06, FKM+07, JMD+02, JCL05, LW04b, LD05b, LZX06, MB00, Maz01, PG04, Pin01, Pin03, PSHP08, PSS+04, PSMB05, RTG00, SG07a, SHD+08, WRP+06, WWL+09, hYDN+08, YS00, ZLY07].

DNA-base [PG04]. do [SRK+00, YJF06]. Dock [BS08, CWV+05]. docked [NMAT01, ZWB09].

Docking [BTLP03, RGZM09, WS02b, AGI+07, AB09, BS05, BS08, CKMC04, CBC+08, CLH+07, CGBF05, CR09b, GZM09, HR08, HLM05, HK02, KCL06, LR03a, LCCL05, MKT04, MM03, MCR08, MHL+09, RK05, Ru07, SBG+09a, TH02, TFN04, TJE03, TP01a, Tot04, VVS07, WRBV03, YK00, Yan04, YKK09].

dodecamer [JCL05]. Does [RY09, RS07a, RS07b, WCK00].

DOIT [SFRS01]. domain [IGNH03, JS07a, OO08, PAT+09, PYCD03, PY05, PC07, TCL08].

domain-averaged [PYCD03, PY05]. domains [GCDL+05, PC05, PC07, SCS07, WCF04]. dominant [LMB08].

DommiMOE [DFWH05]. Donald [Sta00].

donation [HT05]. donor [RM07, SE KS09].

dopamine [FPG+06]. dopants [CM09]. doped [JBGK08, LWLS07, SCP08, WZZ+09, XWL+09]. Doping [SM06, JBGK08].

dot [CLZ+09]. Double [LB05, AZM03, CMJ08, DLRT09, LMG0+09, Won09, YS00].

double-stranded [AZM03]. doubles [IN08, WKYU01, dSVA+09]. doubly [CHRL09, LLD+09]. doubly-linked [CHRL09].


DQ2/DQ7 [KVS+06]. DQ7 [KVS+06]. DQ8 [KVS+06]. drag [YS09].

Dramatic [AM06a, KT08]. dressed [MW09]. driven [MH09, PV03, SVT09, WPS02]. drives [LFS+07]. driving [AM07].

Drude [LLL09]. drug [CMCB08, DHW+09, HS07b, LLW+09, MCR08, PPX01, PFR04a, SPGS08].

drug-induced [CMCB08]. drugs [BLB09, KEH+02, KC01a, SM+08, VGGM05, WM01]. DsbA [CFR06].

Dual [WyLG+09, WLL+03, ZWL+05, mJlZyL07, TST+08, ZZL04].

Dual-level [WyLG+09, WLL+03, ZWL+05, TST+08, ZZL04]. Duan [An006c].

due [Car02, JM07a]. duplexes [BL08, NL08]. duration [CCSJ00].

during [IZA06]. dyad [CHRL09]. dye [BG00, KS05c]. dye-sensitized [KS05c].

Dynamic [SDG02, XLZ08, CC07, CVR08, CEP07, FEV+09, JW06, mJlZyL+08, LLY04a, LG02, LEV+09, QCK01, QCK02, SDL+09, SCC04, SYC08, WM06, XLC08, YCS07, YCYX03]. dynamical [CKW09, EM03a, Kri09b, LDT07, MS03, LPK07].

dynamically [CvG08].

Dynamics [BBG+04, DJB02, KB09, KIM+09, SSBE06, Yos02, ALB09, ATM03, AM06b, BL09, BB05, BWE05, BRDC02, BS01, BG07, CL09, CL09].
E-state [SPGS08]. E1 [YT04]. E2 [RY09]. EADock [GZM09]. early [CMCB08]. earth [JHMB+09, JHMB+11, SO07]. earths [LZZC09]. ECEPP [Sen06]. economic [FZL07]. edge [XWL+09]. edge-doped [XWL+09]. Edited [Sta00]. Editor [JW12, WM12, vLBBR12, Lip00]. editor-in-chief [Lip00]. Editorial [Bro05]. Editors [BFS07, FA01b, FBS09]. educating [BS01]. Effect [CXZ+09, CN05, CEP07, KGL07, Mue01, WMW04, BB08, CPJ00, CPJ01, CGB+09, CSB08, CKT+08, DMJ05, GT03, HK08a, HK08b, KT08, KMM07, KCL00, Kri08, Lee09, LL01, LCA03, Mas04, MZL08, PCS04, RY09, R05, SOOF05, SPDS01, SCG04, SDL07, VM07, WM06, WDX+02, XLW+09, ZY01, ZZS+07, ZWPR+04, CPDZH08, HFS+07, JD09, WMW03, WSC09, vE01]. Effective [OCB02, SBLK01, VBGL+00, BCF+09, CR09a, DPT03, HMWC03, HSWW00, LFK05, MML02, NGTB03, NG04, RPMP03, SG08, VB02]. effectively [SMGE08]. Effects [DXW08, KKH+07, RLP08, WXW08, AD00, ASS+02, BA03, BA04, PAO4b, BPC01, BE07, BDW00, BBI+09, CC07, CKF01, CDPL09, Don08, Dra00, ECA06, FGR07, FHH+01, GWM08, GATG03, GM04, GGLR00, GKT04, HRR05, IC08, JJK+00, JW05, KSK00, LSO8b, LR03b, Loc03, LFR+04, MDA08, PB09, PSF+08, PWFS01, RRCA08, SF07, SL09, SADV00, SURG06, SM06, SN06, SR06, VDM06, WMG07, WD04, Wb04, XY+06, YXZ+04, YH09, Z04, ZWS+02, CM09]. efficacy [KSM05]. Efficiency [IO08, MKGA06, RLERO4a, YA+02, CN03, FMS09, GF08, KK08a, LJ04, LJS05, LKW04, PSMB05, SM08b, SM03, SE08, vLBBR12]. Efficient
efficiently [IGL07, LR06].

[AT02, BP00, BB05, CSJ01, DMZT08, EA08, FL08, FKG09, GHH07, GB04, HMWC03, HTKG08, KMA07, KLC00, Nil09, OD09, Oos09, SAT004, SMM08, TP01b, WM12, YZ04, Ami00, BL09, BP02, BdPRMAI00, CGG06, CIB05, CY09, CY13, DBS08, FG02, GJL08, JB00, JB02, KM00, LSO04, LCKL05, PRSM02, RKA09, SAM06, SSM09, TS05, Tot04, WW03, YXL09, vLB012, FS98, FS00a].

eigenvalue [SSL02].

eight [CWV05].

elastic [AJ03, BED02].

Electric [LTV08, SF07, WMS06, ACD03, BSOB05, CM09, Kar06, LST08, Mar03, OBBS05].

Electrical [KCL00].

electride [LWW06].

electrochemical [Bie04a, Bie04b, Rud05c].

electrocyclization [ZGZX07].

electrolyte [CCCJ09, YSJ09, ZCS04].

Electron [AS00, BK08, BWW08, BLN01, CFS03, FS02, Li01, OON01, PC05, PC07, TKH07, TD06, ZJ07, AEE03, ABF03, BG03, Bac07, BG00, BY06, BLM04, BI06, BRS07, BL00, BAA07, CRC08, CXZ09, CR09a, CHRL09, CKT08, DVP02, DVR03, EL09, FLO07, FR06, FS04, FZL06, FSS00, GKR08, GGA00, GR07, GB03, HLS07, Hr08, HS0W00, IKN08, ITN05, IS07, IN01, Jac09, KS05a, KK08c, Kle03, KFD06, Kri09a, KMM04, Lai07, LMV07, Lee09, L008, LL01, LLL02, LH02, LB05, LB08, MLL06, MGCA07, MGMM07a, MS00, MA09, OKE02, PFB05, PA05, PAS07, QZZ03, RS07a, RS07b, RTG00, SFC04, VC04, VK09, WMW01, WN09, WL00, XWXC08, Yas08, YCXY03, YH09, ZXL04, PC05].

electron-correlation [YH09].

electron-pair [FS04].

electron-repulsion [Kri09a].

electron-sharing [BRS07].

electron-transfer [QZZ03].
electron/four [GYMN07].
electron negativity [dSGC00].
electron negativity [ALC08, BCN07, JV09, VK06].

Electronic [CWWS07, DHH03, FLK07, GGGL05, Hua09a, IME02, KHY00, KMM07, KGD06, LPP06, LT07, OS08, QB05, RPNJ07, SCP08, Wu06, WWS07, XZ05, A03, AEE03, AM02a, AZS04, AGSFA05, ASS02, Bac09, BBG04, CMAGL04, CZF07, CN05, CNN07, CAG07, CR03, CSV07, CTFC08, DD00, FL08, GJL08, GBL05, GM04, HMMS09, HZ09, Hua09b, Kar01, KRM02, KJP07, KIK07, KKK00, Kri09a, KPZ06, LWK08, LWS07, LWZ09, LFR07, LB08, LDD09, LMRF09, MKGA06, MM02, NYH02, PP08b, PMC08, QCK01, QCK02, RRC08, RS05, SS03, XBL05, TD08, TT01, TD06, TDK07, WMW01, WLM05, WL00, YX04, YFR05, YS00, ZY07, ZYS07, ZY08, ZXY09, ZX08, ZL05, ZL07, ZL09b, ZM03, SMK00].
electrons [HIM07, PO03, WJ00].
electroosmotic [YSJ09].
electrophilicity [RUPH06].
electrotopological [SPGS08].
element [Ara04, BHW00, BK08, BH03, BF04, HBW00, HBW01, LI01, SRB06].
elements [ABWT09, ATM+07, ASS+02, EII07, JGH00, RP07b, RRS09, VB03, WL04, vW06]. elevated [TK08]. ELF [SFC04, CFS03, FSS00, PC05, PC07]. ELI [BWW+08]. ELIA [BWW+08].

Elongation [KLM+09, MKGA06]. Elucidating [DBS07]. elucidation [Gz07, GLH+08]. embedded [CEP07, GGLR00]. embedding [Agr03, JNV08, KS02b]. emit[0] [LFR07].

Empirical [CBC+08, LS08c, Mac04, SP05, CVM02, FM00, Gri04, GGK+08, HRBKB03, JCHS07, KK08b, LR03a, LLM09, MB00, RKH03, ZNLI07, VBGL+00].

Elongation [KLM+09, MKGA06]. Elucidating [DBS07]. elucidation [Gz07, GLH+08]. embedded [CEP07, GGLR00]. embedding [Agr03, JNV08, KS02b]. emit[0] [LFR07].

Empirical [CBC+08, LS08c, Mac04, SP05, CVM02, FM00, Gri04, GGK+08, HRBKB03, JCHS07, KK08b, LR03a, LLM09, MB00, RKH03, ZNLI07, VBGL+00].

Energies [CRSB03, BP02, BWE05, BLL+06, BE07, BDW00, CHA+07, CCK01, CPML08c, CG05, DB07, DMZT08, FOL+04, FJP07, FKU+05, GS04, GKTS04, HT05, HYA02, Hol05, IIO8, JK+00, JCL05, JD09, KCK+08, PBF07, SLH09].

Energy [CBH+03, HFHL06, IN08, KLS02, MSF+08, NK06, SS07, WM12, dSR08, AMR04, AJO3, AB04, AE06, AM06b, ABBC01a, ABBC01b, AGSFAL05, BM07, BCI05, Ber03, BL05, Blo04, Bo01, BRLS08, BRLS12, BACJCT01, BF07, BLB09, CC09, CN03, CCB04, CY09, CY13, CJW+09, Chi03, yCkhN08, CV09, CMGDA+07, CA04, COL+06, DLD+02, DLRZ09, DMJ05, DK01, EGSG00, FSS09, FM07a, FJK+01, FZL+06, GZL02, GMA04, GLMV09, GadGM08, GG09, GC04, GS02, GS03, GPS06, GB02, GWS+02, HKMS01, HP01, HR08, HMOG07, IGNH03, ILKR09, IGL07, IPN06, IPN07, Jac09, JMD+02, KGN07, KN04, KKC05, KUB07, KB09, Kob03, KCO1b, Kri09a, Lab08, LR03a, LMK01, LF04, LFZS04, LJ04, LBG08, LKW04, Lu09, MG06, MCF05, MAF+07, Mza08, MH09, MGJAARC00, MGLO03, MRS+07, Nak02, NKIS02, NA06]. energy [OD09, OFB08, ONHN00, OKH+02, OV03, Oos09, PSC+01, PMGL03, PK04, PAT+09, PMPGP05, Qua01, RP07a, Rao00b, Rap06, RSE07, RRC08, RWBH09, RHL09, SOOF05, SPD01, SKG00, SPL+02, Sch03, SMGE08, Sen06, SRC03, SSM08, SY09, SG07b, SSMW09, SMD02, SJW09, SSBE06, TJE03, TGGP+00, TCR+02, UTH+03, VE09, VM02, Vya01, WL02, WD04, Whe08, WHF08, XZZ04, YXC+07, YZ04, YHD+06, ZCZ03, ZZ08, ZGXX06,
vEMK01, vLBBR12, Hir08. Energy-based [KLS02, MSF’08]. Energy-consistent [SMD02]. Energy-transfer [MAF’07]. Energy/one [Oos09]. Energy/one-step [Oos09]. enes [PWFS01]. Engine [MVL’05]. Enhanced [KG02, DAK08, NYTH09]. enhancement [AB08]. enhancements [AM06a]. enkephalin [ZCL09]. Enones [SLRC01]. enough [VGGMM05]. Ensemble [Blo04, BSC’01, EMP07, O006, SM08b, SM03]. ensembles [GLD08, Ike04]. Ensure [FKFG08]. Enveloping [BHH’09, CV09]. Enthalpies [EB04, WC04, BE06, RM00, TTBM09, VGGMM05]. enthalpy [OVMV04]. Entire [ZAT07]. entropic [CBC’08, FGR07]. Entropy [DHF’05, HDF’07, HTKG08, KKH’07, LM03, RK05, Ruv07, STSF02, WG02]. Enumeration [AL01]. Envelope [BHH’09, CV09]. Environment [DFWH05, DPM09, GT03, HFS’07, PPM05, GBL’05]. Environmental [CMGDAC’07, FGR07, MDA08, TP01a, VW03]. Environmentally [EDAJ04]. Enzymatic [PCM09]. Enzyme [CFER04, Fie02, GGLR00, GS04, MDA08, Pin03, TDH06, VB09, ZL09a]. Enzymes [BS06, CPU09]. Epimerization [BBSS06]. Epitope [SHBD05]. Epitopes [KVS’06, SHBD05]. Epoxide [Owe05]. Epoxides [OY01]. Epoxy [OY03]. Epoxy-amine [OY03]. EPR [SN06]. Equation [AMR04, ABWT09, BHW00, BH03, BF04, BF07, BR01, F00b, H055, HBW00, HBW01, SAT04, TW03, Vas02, Vis02, Zho06]. Equations [Bie04a, CF04, DOSG06, Har04, Kvh01, LPK07, LMJ02, QNF09, R107, Rud05a, Rud05b, Rud05c]. Equilibrated [CA07a]. Equilibration [SDCG02]. Equilibration-Morse [SDDC02]. Equilibria [FGR07]. Equilibrium [KSTC01, BGP09, ECA06, KBLP09, LS08b, MMLC05, PAM08, ST04, VMG07]. EQUIPATH [Kli01]. Equivalent [ZZY07, WBSR03, ZZY08]. Equivalents [RCJ02a, RM00]. ERE [MCF07]. Erratum [ABBCC01a, An05b, An06a, An06b, An06c, BA04a, BRLS12, CY13, FS00a, HNW01, HBW01, HK08a, JHMB’11, KWK’02, LFSB03a, LR03b, NBTN04a, PCO’07a, PW07’04, RS07a, TX01b, WB04a, WB05, WMW04, WWC05]. Error [IO08, KMA’07, Kob03, Mas04, MD04, RS05, Rud05a, Rud05b, Rud05c, TBS09, V0K’08]. Error-ranked [TBS09]. Errors [CS03]. Erythronic [vDSSV04]. ESFF [SYY’03]. Essay [BHTCG07, FK07b, GR07, Kut07, MGCA07, Nye07, Sut07, Sim07, Tru07]. Established [SB01]. ester [TH02]. Esters [POJ01]. Estimate [KC01b, YZ04]. Estimated [ZM09]. Estimates [GC04, H055, MD04, SY09]. estimating [HDF’07]. Estimation [DHF’05, ZW09, CV09, DDD09, HTL09, KC01b, PYEA03, Lab08]. estimators [GJL02]. Estrogen [FKU’05, KBK’01]. Ethane [DGD’05]. Ethanes [WyLG’09]. Ethene [Ang09]. Ether [GLRL02, WD04, WLL’03, YLL’08]. Others [ACLD03, LCCBA03, LCGA03, LCA03, ZWY’09]. Ethyl [KKH’07]. Ethylene [TBG00, BSJ01, Hir08, NTH00, SBB02]. Euclidean [RRS09].
EUDOC [PPXP01]. Euler [SG01]. evaluate [GGB07a, GGB07b, LF04, OSH03, TSSGS07]. evaluated [ABBC01a, ABCB01b, Bo01, Qua01]. evaluating [FO08, Con02]. Evaluation [BMLV04, DR07, KSM05, NMAT01, OYH09, VKP08, YSJ09, Ano05b, AGSFAL05, CGG06, CAG07, DSR07, DBS08, ESP04, FMAMVK06, FKZ09, GGA00, HMWC03, JSHG07, KJWV08, KH06, LMV07, LYS08, MSH06a, Mor02, PRS04, Sha05, VP02, WL02, Yan04, YS08, CBC08, GKT04, OGH05, ZSK07]. evaluations [SF05]. Evans [SRK00]. EVEBAT [CZA03]. Even [CVVB04, CC07, VVBV02]. Even-tempered [CVVB04]. evidence [BLO02, IO08, SFR07]. Evolution [BMLV04, DR07, KSM05, NMAT01, OYH09, VKP08, YSJ09, Ano05b, AGSFAL05, CGG06, CAG07, DSR07, DBS08, ESP04, FMAMVK06, FKZ09, GGA00, HMWC03, JSHG07, KJWV08, KH06, LMV07, LYS08, MSH06a, Mor02, PRS04, Sha05, VP02, WL02, Yan04, YS08, CBC08, GKT04, OGH05, ZSK07]. evaluations [SF05]. Evans [SRK00]. EVEBAT [CZA03]. Even [CVVB04, CC07, VVBV02]. Even-tempered [CVVB04]. evidence [BLO02, IO08, SFR07]. Evolution [BMLV04, DR07, KSM05, NMAT01, OYH09, VKP08, YSJ09, Ano05b, AGSFAL05, CGG06, CAG07, DSR07, DBS08, ESP04, FMAMVK06, FKZ09, GGA00, HMWC03, JSHG07, KJWV08, KH06, LMV07, LYS08, MSH06a, Mor02, PRS04, Sha05, VP02, WL02, Yan04, YS08, CBC08, GKT04, OGH05, ZSK07]. evaluations [SF05]. Evans [SRK00].
Extending [GCD04, MFB04]. extensible [SYY*03, GBL*05]. Extension [CR09b, FBL008, GY08, TBGRJ04]. Extensive [JW12, LB08, SLHW09, YXL*09, ZL05, SMG09]. external [CM09, EC06]. extra [LW07], extra-valence [LW07]. Extracting [HM02], extraction [OD09]. extrapolated [KSTC01, Var09]. extrapolation [MO09, MC06, PSC+01, PJF+03]. extremal [ZZ08]. extremely [GFS05]. Eyring [Nye07]. Fac [CRC*08, FO04, Gog08, HYA02, HZ09, Hua09a, IV04, KS05a, KBL08, Mar03, RB01, STC*08, UTT*04, WLLS04, WLL07a, XL*02, ZLLS06b, ZL09b, HK07, KS05a, RF606, SOOF05, Sha02, WDWS06, WYW03].

Facility [SWZ04]. factor [LMD09, WL00, XSHC06]. factorization [EC06]. factors [AST06, SBH02, TP01b]. FACTS [HC08]. family [CFS*09, DMC05, NAT07, WTKM06]. FapydG [SHD*08]. farnesyl [SFR07]. Fast [JBB00, JBB02, JSHG07, NG04, RS08, SYC03, SFC04, Am00, AMK03, An05b, CS02, CRG01, CHMI05, CZA03, GY08, GKK07, HH04, HLM05, Ish04, KM00, KLM*09, KvGH01, KH06, PS04, RK05, San01, SCC04, Sha05, TRS02, VP02, WCC08, HC08, LZ05a, VLH*05]. faster [SF05, AM06a]. faujasite [TLOG00]. faujasite-type [TLOG00]. FB [DHW*09]. FB-QSAR [DHW*09]. FBP28WW [PAT+09]. FDS [TJE03]. Fe [BTP09, HLLN06, HYR06, KRLD09, AGK03, KT08, DF04, Mck07a, Mck07b, NyHN06, NHN06, PL08]. feasibility [MWE02]. feed [SJJ*04]. feed-forward [SJJ*04]. feedforward [LJZ*07]. Felix [An06a, An06a]. FeMo [Mck07a, Mck07b]. Fermi [Kri09a, PYC03, PYS05, PC07, PL08]. ferrocene [Kan07, MBP09, ZZS*07]. ferromagnet [TD08]. ferromagnetism [SK08]. FeS [Mck07a]. Feynman [RLER07]. Field [MO01, AS06, ACLD03, An06b, An06c, ATBL04, BWF*02, CLP09, CLYL09, CPM03, CM09, CGB03, CLA*00, CR02, CS05, DvG00, DPT03, DRMD03, DFWH05, DMLJ05, DGI*08, DWH*08, DWC*03, EBD*01, FHR07, FBBD06, FAR02, FM00, GZL02, GMA04, GRO*03, GGK*08, HP01, HGMB04, HXL09, HIM07, HNL08, HMOG07, IDMC09, IT03, IKYM09, JS07b, JCL05, JM07b, JFG04, KB02, KSB*02, KS06, KAR06, KFN08, KTA03, KOFF05, KLB03, KYT*08, KOML08, KDSV02, KVL*04, KBN02, LLO0, LST08, LTV08, LFZS04, LAT05, LH05, LLM09, MT03, MB00, MM05, MP03b, MBC08, MMY07, MSR04, MRC03, MHJS06, NUH02, NCO*05, OYH05, OMN08, ONH00, OKH*02, OVMV04, OB09, PB04, PBM04, PS09b, PHF*03, PWFH*04, Pom04, PHH*08, POJ01, PB05, RSN*02, RK03, SF07, SO09, SDL*09, SdjG01, SAS05]. field [SDCG02, SSS*09, SYY*03, SHK*05, SP05, SK05, TAP07, TTB01a, VS*03, VCM01, VTT*08, WK01, WWC*04, WWC*05, WZW*06, WMS06, Wil01a, Wil01b, XLT07, YCYXY03, ZWC*09, vDSSvA04].

field-based [DMLJ05]. field-derived [WMS06]. field-induced [CGB03]. fields [ABA04, Car02, EBD*01, HRBBK03, LLM08, Mac04, MFB04,
OSH03, PK04, PB02, RP07a, RLER04b, RG08, SL09. files [FJP07]. fill
[RRZA08]. find [HQ02, WS07]. Finding [BS01, Qua07, GF08, Rao00b]. fine
[VK04]. fine-grained [VK04]. fingerprints [LHJ06]. Finite
[Ell07, MO01, AB09, ALKH04, BHW00, BP01, Beo4a, Beo4b, BF04,
DRMD03, Der09, GM04, HBW00, HBW01, KGD06, PZS04, RP07b, Rud05a,
Rud05b, Rud05c, VZM08]. finite-chain [Der09]. finite-difference
[Bie04a, Bie04b, Rud05a, Rud05b, VZM08]. finite-temperature
[KGD06]. finite [LDC07]. First
[CS01, HZX04, Hua09b, TK08, WZZ09, ZDY08, ZHZ08, ZHL08, ZHW09,
AD00, BP03, CJK02, EBL08, FO08, GJL08, GD09, JPCA08, KS08, LWZ09,
Mck07b, MLJ03, Rud05b, VP08, WLX05, XWL09, KSB02].
first-order [Rud05b]. First-principle [CS01, HZX04, Hua09b, TK08, WZZ09,
AD00, BP03, KS08, LWZ09, Mck07b, MLJ03, Rud05b, VP08, WLX05, XWL09,
KSB02]. first-row [AD00, BP03, LWZ09, Mck07b, MLJ03, Rud05b, VP08,
WLX05, KSB02].
first-row [AD00, BP03, LWZ09, Mck07b, MLJ03, Rud05b, VP08,
WLX05, KSB02]. fitted [YOB08]. Fitting [KC01b, MCF05, Wei08].
finite [SBH02, Van02a].
fixed [SBH02]. fixed-composition [HM06]. Flex
[GCD04]. flexibility [BL08, BCP04, KG02, KTA03, MH08, 0V03].
Flexible [COS01, NGTB03, YK00, AGI00, AGI07, AJ03, AHGK09, BS08,
CCL06, CMK04, CLH07, DDKV07, GCD04, HW09, JNV08, KOFF09,
MH08b, SSBE06, TFN04, TP01a, Tot04, VLH05, vEMK01, vE01, TJE03].
flexible-backbone [AHGK09]. flexible-ligand [HW09].
flexible-protein [HW09]. Flooding [LSG06]. Fluctuating
[OR05, KMH02, PB04, PMB04, Yos02]. Fluctuation
[MHW04, PC05, SLK01]. fluctuations [AZS04, WMGK07]. fluid
[BCIB05, CLC09]. fluorene [CHA07, YFR05]. fluorene/pyridine
[CHA07]. fluorene/carbazole [YFR05]. 
fluorescence [CHA07, MAF07]. fluorescent [DHM03, NAT07, VSW03, XZ05].
fluoride [BGC07, IV04]. fluorides [KS05a]. fluorinated [CUS03].
fluorobenzene [ZTP08]. fluorobutanal [NSB08]. fluorocarbons
[JARM02]. fluoroglycine [HS00]. fluoromethylene [ZLL04a]. flux
[DAK08, RKA09, Rud05a, Rud05b]. fly [KMA07]. FMO
[FOK04, FKL06, KIM09]. FO [Gog08]. focal [KK08]. Fock
[RSS07, TW03, WMW04, AKN07, Bo00, Cu04, DD00, GADG08,
HDD04, MS00, MBW03, PFJ03, PVdJB00, TOY02, UHN09, WMW03,
Wei08, YH07, vDSSwA09]. Fock/Kohn [RSS07]. Focus [Mat03]. focusing
[KBK01]. fold [DB06, ZM06]. folded [CP08, GB04]. Folding
[HEP02, ADM06, CCC03, DvG00, HGO8, IM06, JS07a, JIK09, KH05, ML04,
MO09, Mei02, MWE02, RLP08, V00, V04, VGO07, ZPO3, dSR08].
folds [BS01, ZS04]. following [DLD02, LMO09]. For-Gly-NH [PC00].
For-L-Ala-NH [PC00]. Force [CLP09, JCL05, OSM08, OBT09, SO09,
SL09, ZWC09, AM07, AS06, ACLD03, AB04, A065b, A066c, ATBSL04,
CLL09, CA02, CP03, CLA00, CR02, CS05, DvG00, DGI08,
DWC03, EBD01, FBSD06, FAR02, FM00, GRO03, GGK08, HP01,
HGMB04, HXLS09, HRBKB03, HFSD03, HNL08, HMOG07, IDMC09, IT03, IKYM09, JS07b, JM07b, KB02, KSB*+02, KS06, KFNH08, KTA03, KOFF09, KLB03, KYT*+08, KI03, KOML08, KDSV02, KVL*+04, KBN02, LLM08, LL00, LMO*+09, LH09, LAT05, LH05, LLM09, MT03, MB00, MM05, Mac04, MFB04, MLC05, MBC08, MMY07, MSR04, MRC03, MHJS06, NCO*+05, NMAT01, OYH05, OSHS03, ONHN00, OKH*+02, OVMV04, PB04, PMB04, PK04, PS09b, PHH*+08, POJ01, PB02, PB05, RP07a, RNG03, RI07, RG08, RK03, SDL*+09, SDvG01, SAS05, SDCG02, SF05, SSS*+09]. force [SYY*+03, SHK*+05, SP05, SMM*+08, SK05, TAS07, TTB01a, VSW*+03, VCM01, VTT*+08, WK01, WWC*+04, WWC*+05, WZW*+06, Wil01a, Wil01b, XLT07]. Force-field [CLP09, OBT09, SO09, HGMB04, IDMC09, KLB03, MBC08, NCO*+05, OKH*+02, OVMV04, SP05, VCM01]. forced [CAG07, LPB03]. force-field [Adc04]. forces [BCF*+09, BH03, HNWF07, HNWF12, JS07a, LPB03, PK05, RLP08, WB04a, WB04b, WB05]. Foreword [DF08, Fre00, FJ02, FH06, FS07, Gad03]. form [AT02, Bac07, BRS01, CR02, LC07]. formaldehyde [WCL05]. formalism [AS00, FLGW00, YCXY03]. formalisms [CF06]. formamide [HIN09, Pac06]. formamidine [WJX*+08]. format [TDK07]. Formate [ČJPZS08, NK06]. Formate-Lyase [ČJPZS08]. formates [CUSS03]. Formation [JM07a, RAGLL09a, RAGLL09b, BE06, BMTFR08, CS03, EB04, HIA03, JWB05, KLB02, LLA01c, LYZ*+08, Nee03, RCJ02a, RM00, TT08, TTBM09, WC04, WX09, ZZW09, dOMSL01, JKM08]. formed [LLW02, LSW*+01]. formic [Pac06]. forming [PP08a]. forms [SPT07]. formulas [Ish02, Tor02]. formulation [BF07, Cul08, PK05]. formylnyl [GSB09, HJCP01, PFC03]. formylglycinamide [HRBKB03]. forward [KM07, SJJ*+04]. Four [SH02, FJ08, GPS06, Lai07, PVdJB00, PV03, SBH02]. fourth [Lai07, SBH02]. four-centers [GYMN07]. Four-component [SH02, GPS06, PVdJB00, PV03]. four-index [PVdJB00]. four-membered [FJ08]. Fourier [BWP07, CGG06, HLM05, TYN05]. fourth [Bie04a, Rud05a, Rud05b, Rud05c]. fourth-order [Bie04a, Rud05a, Rud05b, Rud05c]. FPT [BPC01]. fractal [Pan07, TT08, XOW*+00]. fractional [MGLO03, SM08b]. fragilis [SDM02]. Fragment [DHV*+09, CFK08, DPM09, FOK*+04, FKL*+06, FII*+07, FKU*+05, FKM*+06, FKM*+07, IK09, KIFK07, MLG04, MLL08a, NYK*+09, NGB03, NG04, OO08, SG07b, ZMZ09, KIM*+09]. Fragment-based [DHV*+09]. fragmental [CSB*+03]. fragmentation [Gor01]. fragments [AM09, DWN01, DPRR05, KS01a, LV08, NG04, PBF07]. Framework [JGVF05, CR08, EA08, FS04, TASN07, Tie09]. Framework-based [JGVF05]. Franck [Ama02a, LMCD09, TP01b]. Free [DLRZ09, GS03, JMD*+02, MH09, PMGL03, YXC*+07, AM06b, BG00, BWE05, BLL*+06, BCI05, Blo04, CN03, CM09, CY05, CY13, Chi03, CV09, CCK01, CMGDAC*+07, CG05, COL*+06, DMJV05, FSM09, GZL02, GMA04, GLMV09, GG09, GC04, GS02, Gra07, GWS*+02, HKMS01, HR08, HMOG07,
ILKR09, IGL07, JZD^+09, KDG^+09, KAS^+07, KKC05, KUB07, KB09, Kob03, KK01a, Lab08, LR03a, LF04, LSW^+01, LWK04, MG06, MT03, MGL003, MRS^+07, OD09, ONHN00, OKH^+02, Ov03, OVMV04, Oos09, PK04, PAT^+09, RSE07, RWBH09, SOOF05, SAM06, SKGS00, STSF02, SBL05, SSM08, SY09, UBDPJ04, UTH^+03, Vlh^+05, VE09, VGDSU08, VM02, WHF08, XLT07, YZ04, ZMZ09]. Free-base [SBL05]. Free-energy [JMD^+02, AM06b, CY09, GMA04, ONHN00, RWBH09, SKGS00]. Free-energy-driven [MH09]. freedom [DHF^+05, MZL08]. freeze [BME05]. freeze-and-cut [BME05]. frequencies [BRV^+07, Han01, Kle03, KBN02, LMB08, PZWG^+04, WM04, Zwpr^+04]. frequency [DF06, DR09, My08a, VSW^+03, YH07]. frequency-dependent [My08a, YH07]. frozen [AEE^+03, GWS^+02, JNV08]. frozen-density [JNV08]. fructose [MRS^+07]. fuel [CCCJ09]. Fujitsu [KSY^+00]. Fukui [DVP^+02, FS04, TSSGS07]. fulfillment [RLER07]. Full [PRSMV08, GD09, IR03, KGD06, RS08, ZCZ03]. full-atom [RS08]. fullerene [CHRL09, CTFC08, GYCZ04, GKK09, Kan07]. fullerene-dizincocene [GXK09]. fullerenes [GZ07, GM01]. Fully [GWM^+00, XZZ04, WTKM06]. function [Bac04, BS05, BdPRMAI00, CFS^+09, Che01, Banking08, CPUGD09, Con02, DMZT08, DP03, FSS00, GCB03, GS09, GdAcV^+07, GPN01, Hmwc03, HZ06a, HZ06b, ILB03, ILKR09, Ish04, KK08c, Kni00, KFD06, LR03a, LHI09, Lbt07, MP03a, MML02, MY08b, Nak07, NKIS02, PP08b, PA05, PAS07, SFC04, SJW09, TLKT00, TW03, TJE03, TT05, TSSGS07, VVS07, YLL^+09]. functional [AAP00, AB00, ABYM08, ASY01, Bac09, BP01, BE09, CLP^+05, CKF08, CRS05, CR08, CSB08, CPML08a, Cul04, DVP^+03, ECM^+03, El09, FCW06, FZL07, FG02, GHLK^+02, GM01, GLRL02, Gri04, Gri06, GBBH09, Ha08, Han01, Hnwf07, Hnwf12, Hol05, Ion07, Ib04, ITN^+05, IS07, JFG04, JCHS07, KGL07, KSS08, Kwk^+01, KKK^+02, Kzw^+05, Kri09a, LRI^+02, LWK08, LMB08, LMGR05, LLS03, LWH06, LKT04, LF02, LLZL09, Ldl^+09, LZF^+09, MW09, MSBS01, MW00, NTH09, Nat07, OKE^+02, PSF^+08, PU09, PDS01, QZZZ03, QZL^+04, RB01, RK04, RDM^+08, RR05, RZWS07, SH07, SZT08, SPT^+03, SP07, SLRC01, SS07, SW06, TBG00, TST^+08, TKN^+08, TKH03, Van02b, VMA03, VL00, VB09, WRP^+06, WB07, WZY04, WMRW^+01, WL02, WCW08, WCHW09, WM04, WSC09, WCL05, WXYY07, WM01, XYN^+06, XB08, XWC09, XL02]. functional [XPW09, YYY07, YLL^+09, ZLL04, Zho06, ZM03, vGGB00]. functional/continuum [LRI^+02]. functionals [BP03, DF04, Han01, Ion07, JPCA08, Krm^+02, KS01b, PJPjdPRMI07, SCF^+09, WL04, YTH01]. functions [AE06, Bac07, Bou00, CGB03, CGSdST06, DVP^+02, GFS05, GLD08, GS07, GBJ03, IT03, MLL06, My08a, Nuh02, OFB08, PFB05, RHL09, Ruv07, SS00, TS05, TD06, WG02, YH06, ZMZ03]. Fundamental [LMB08]. fungal [LPP06]. funnels [HEP^+02]. furfural [COMR^+04]. Further [GPK05]. fusion [CRGN07]. fuzzy [ALTB06, EKB02a, RLA01]. FVII [PDP02].
G [AGI+07, Kró03, XWC09]. G** [Wib04]. G-protein [XWC09]. G. [CSD05, Sim07]. G2 [RY09, ZKZ+07]. GA [HSMT04, HSMT04, LLL+08]. GA-MLR [HSMT04, LLL+08]. gadolinium [AB00]. gain [HP05]. gains [NYTH09]. galabiose [RSSKB03]. galactose [RSSKB03]. GAMESS [UKNS01, UKN04]. gamma [Ish04]. gap [KUB07]. gap-free [KUB07]. Gas [BAL+01, POJ01, CPJ00, CPJ01, DR09, EGSG00, JJK+00, JHZ09, KSB+02, KTO8, KKH+07, LRI+02, Lee09, LZA02, LB05, LXS08, MFB04, Mas01a, Mas01b, MM02, Pan07, PV07, wQZsLyZ02, RRS06, ROG00, SMGE08, STSF02, SMKM00, SK05, TDH06, UCT+03, UNM+01, WD04, XKKL03, XKG+05, YQQH09]. Gas-phase [BAL+01, POJ01, JHZ09, KKH+07, Lee09, MFB04, wQZsLyZ02, TDH06, UCT+03, XKKL03, YQQH09]. Gaseous [WDWS06, PG01]. gases [SRB06]. gauge [Ish03]. gauge-including [Ish03]. Gauss [DBS08]. Gaussian [TdMSD+08, CMJ08, Duk01, EDW07, GC02, HDMS05, HdS06, HD06, IO08, Leho06, Lu09, MV06, MY08a, RC04, TW03, WTKM06, YJF06]. Gaussian-2 [RC04]. Gaussian-type [Leho06, MY08a, TW03]. GAUSSIAN94 [Kli01]. GB [GC04, WHF08, GWS+02, YJF06]. GB/SA [GWS+02]. Ge [LLXS02, WDXS06, CJS+03, LLXS02]. GeD [WDX+02]. GeH [LLXS02]. gemcitabine [PFR04a]. geminal [TT05]. geminals [TT01]. general [AM07, BR01, DGI+08, EBD+01, JM07b, KSB+02, LJS05, NUH02, RG08, SAM06, TZX01b, TZX01a, WWC+04, WWC+05, XYN+06, BR07, EA08, FGW00]. generalizable [Kyt+08]. Generalized [ADM+06, ILB03, AB08, BC06, Bud07, CPJ00, CF06, Cul08, DLG00, FOL+04, FL08, FC06, GZL02, ION07, Lab08, LFSB03a, LFSB03b, MTE04, MCM04, OCB02, SHH07, Töt04, XL02, YF06, ZGFL01, dGWH01, BPCD07, FOK+04]. generate [BWT+02, CA07a, BAH+02]. generated [Kri09a, LAH+03]. generating [AMR04, CA04]. Generation [RLER07, BS05, BA+02, Ell07, EKB02a, JJBJ00, JJJ00, KSB+02, LS08b, MM03, PVJB00, PABK03, YJF06]. generator [Fau01, HDBD04, LN01, VW00]. generic [vCkHnY08, Yan04]. Genetic [LSY02, MM07, YL06, BMTSC01, CKMC04, HHJ03, HWDB03, HMSM06, KOFF09, LJS05, SPT07, SBH02, TP01a, WK01]. Geometric [CSRST04, ZTTS09, Est07, LDL+09, RSN+02, ZXY08]. geometrical [GRC0D0, Kle03, MLL+08a, PJB+07, SCF+09, GCD+04]. geometries [BB08, Han01, IZA06, JCHS07, KKY01, KJP+07, WB07, Wib04]. Geometry [Bud07, LHP01, RK04, VMF+03, BP00, Bie04a, BM00, Cri04, GPSP06, HHHB00, IZA06, KKG+09, KHF+09, Kle03, LJ04, MBP09, MW00, PO03, Pul05, RON02, SCP08, WPS02, ZSS+07]. GEPOL [PTC01]. Germanium [LLXS02]. GEP [HFS+07, NINAT+07]. GGA [DDBP09, Gri06, RLDI09]. GGA-type [Gri06]. GIAO [FO04]. Gibbs [EGSG00, HR08, IGL07, Lu09, SM08b]. Gilbert [GR07]. Gillespie [RMP01]. give [JJK+00]. glasses [NA06]. Global [CZB07, FTLV01, JHZ09, CS02, CMBC08, LS05a, RUPH06, SE08, TSSGS07, TSSSG08, WS02a, WG02, UK04]. Globally [PAS08, TP07]. Glu441
[PCS04]. glucans [CMD+04]. glutamate [FTLV01]. glutamic [ZZY07].
[WC08]. Gly [PC00, VKP+08]. GLYCAM06
[KYT+08, SDL+09]. glycinamide [LB05]. glycine
[BA03, BA04d, BA04b, GAIVB01, GSB09, GKT04, KAS+07, LB05,
LSW+01, MOP+07, PG01, ROG00, ZW09]. glycol [Pin01, RR05].
glycol-lesioned [Pin01]. glycosidase [BMTFR08]. glycosidase-inhibitor
[BMTFR08]. glycosidase-substrate [BMTFR08]. glycosidic
[SO09, SDL+09]. glycyl [KOML08]. going [CCK01]. gold
[BR04, CZ05]. gold-capped [CZ05]. GolP [IDMC09]. good
[XWC09]. GPCR [XWC09]. GPCR-CA [XWC09]. GPU [NYTH09]. Gradient
[SE07, DLD+02, DSR+07, FRLN09, GMA04, ION07, Ish02, IPN07, LST08,
TNS00, WL02]. gradient-based [FRLN09]. Gradients
[WM12, BWP07, HHS+05, IK00, KBT03, LJ04, SSMW09, vLBBR12]. grain
[PSP08]. grained
[CP09, DR07, DJB02, HXLS09, MBC08, SBJ08, VSK+04, VTT+08, WWL+09].
graining [CA07a, EBAN07]. grand [EMP07]. GRAPE [Höf05]. graph
[CLZX09, GMGM07a, Pog03]. graphene [KK08c]. Graphical
[LD05b, DPDG05, JKI08, KMH02, KBT03, LW04b, LZ06, Pra01, YNW05,
hYDN+08]. graphically [GS09]. graphics [FEV+09, SPF+07, YAS08].
graphe [BFC+09, EKO+01]. Gravitational [WS02a]. greedy [TGD05].
green [DHM+03, XZ05, KK08c, KFD06, ZM03]. grey [XLC08]. grid
[ALB09, CG06, Pom04, RSN+02, RKA+09, SKSH07, STH02, WL00,
WRBV03, YK08]. grid-based
[ALB09, RSN+02, RKA+09, SKSH07, WL00, WRBV03]. GridMAT
[ALB09]. GridMAT-MD [ALB09]. grids [Bie04a, SFC04, TTHN01].
GROMACS [KVF+07, LSG06, VLH+05]. GROMOS
[CLWL09, CHB+05, LH05, OVMV04, SHK+05]. GROMOS05 [CHB+05].
GROMOS96 [SDvG01]. groove [BCP03]. grossular [ZWTP+08].
Ground [HM10, PO03, PSS+04, BBI+09, CWY09, FCW06, FDSA00, IR03, Kri09a,
LMK01, ZOJ+06]. Ground- [PSS+04]. Ground-state
[HM01, Kri09a, LMK01, ZOJ+06]. group [ATBLS04, CQ04, DVRP+03,
EL07, EB04, JWB05, JGH00, KBT03, LW07, MBM+00, MA05, RCJ02a,
RZWS07, RKH03, SGP09, SN00, TD06, dSCG00]. groups
[BE09, EB04, FJ08, Van02a, WSC09]. growing [Qua07]. grown [WHH+06].
Growth [TDK07, HMK02]. Grubbs [YXC+07]. Grubbs- [YXC+07]. GS
[MH09]. GS- [MH09]. GTO [CBG03, RLRE01]. guanine
[EL07, GWL07, HHWG08, JMO7a, KKM04, MSB01, MHS05, SMK00].
guanine- [KHS05]. guanine-cytosine [KKM04]. guess [Qua07]. guest
[LMM04, Oos09]. GUI [JKII08, SD09]. Guide
[SH08, Woo01, You11, Bic09]. guideline [MWE02].

H [AGI+07, BAL+01, BPC01, BL00, CPJ00, CS01, DRAS04, GSP06,
HYA02, IN08, IS03, LDMR01, LMK01, LXX02, LW04a, LYZ+08, LMO09,
Mas01a, Mas01b, MGLL03, SLL+04b, TYNO5, UCT+03, WDXS06, XDS06a,
ZZL04, ZZL04+, dRLMS00, CPDZH08, CJW09, CGB03, DLD02, Don08, EdiVR03, Gog08, HK07, IIS06, LC07, LDC07, LLXS02, LB05, LN01, LLL07, LS05b, LMO09, MR02, McD08, MY08a, NL08, OO04, PGRNG03, PRSMM03, PVO7, RFSS06, RWBH09, SOOF05, SEKS09, SLL04a, WDS06, WTKM06, Wi008, Wi01b, WX02, YTY07, ZY01. H-bonded [LB05, McD08, NL08]. H-NMR [AGI07]. H5N1 [DLRZ09]. Hairpin [ZHH09, CJW09, IGNH03, LHI09]. Hairpins [IGNH03, Der00]. Half [FMAMVK06, PS03, PMM06]. Half-numerical [FMAMVK06]. half-reaction [PS03, PMM06]. halide [RC04, CW02]. halides [AB00, LYK04, LSY02, ZJM07]. Hall [SPGS08]. halo [TT02]. halo-hydroxymaldehyde [TT02]. halocarbons [NYK09]. haloacid [NYK09]. haloalkane [CS03]. halogen [BS03, FHF01, GGP09, LZF09]. halogen-bonded [LZF09]. halogenated [STC08, TZX01b, TZX01a]. halogens [TBGRJ04]. halothane [TZX01b, TZX01a]. Hamiltonian [FGR07, FdBG08, MR02, SAM06, WZPR04]. Hamiltonians [CV09]. hand [DFGB09]. handle [GCD04, GM04]. Hansen [BBG04]. Haptic [MR09]. hardness [PRS04, TSSGS07, TSSSG08]. hardware [ATMK03]. harmonic [CLP05, Ish02, TFN04]. Harris [Cul04]. Hartree [WMW04, AKN07, Bonou00, Cun04, DDO00, GAdGM08, MS00, MBW03, PFJ03, RRS07, WMW03, Wei08, YH07]. HAsXH [LS08a]. having [Wd00]. haystack [BS01]. HBCC [BAL01]. HBP [OYH09]. HBr [SLL04b]. HBSITE [OYH09]. HCCX [Mar03]. HCI [BL06, WDS06]. HCO [JPF00, dRLMS00]. HCO-L-SER-NH [JPF00]. HDMR [LRGW03, LAR03, LSHR04]. head [HWSN01]. heart [TKH07]. heartland [Sha07]. heat [DOMSLL01]. heats [CS03, JWB05, RCJ02a, Wd09, LLA01c]. heavier [ZJM07]. heavy [BPC01, SL09, WL04, ZX08]. heavy-metal [ZX08]. HeC [Var09]. Helical [CPML08b, Van08, Dd00, KF02a, LC09, PCO07b, PCO07a, ZALMG03]. helicenes [VKP08]. helices [IGNH03]. Helix [BRDC02, JS07b, LJo7, PP08a, YS00]. Hellmann [RLER07]. hemagglutinin [DLRZ09]. heme [ATBS04, MBM00, OYH05, RGZM09, RZWS07]. hemicarcerand [LMMM04]. hemoglobin [MLE06, SO07, Sen06]. Henry [Sch00, TLOG00]. hept [STC08]. hept-C [STC08]. heptafluoropropane [MDC07]. heptagon [STC08]. heptagon-containing [STC08]. heptapeptide [OM04, YA02]. herbicidal [XYN06]. hERG [MCR08]. Hess [YH09]. Hessian [KK01a, NKIS02]. Hessian-free [KK01a]. Hessians [ASWG07, Cha07]. heteraromatic [LLL09]. heterobimetallic [RD00]. heterochiral [ZO07]. heterocycles [FGS00, MGMMM07b]. heterofluorones [CZH07]. heterogeneity [HS01, ZSC05]. heterogeneous [FCK08, ZCS04]. heterohelicenes [LC09]. heterolevel [EA08]. heteropentalenes [CDL06]. heteropolymers [SBJ08]. Heuristics [DMC05, DLHC06, CAGR08, IZA06]. Heusler [GD09, KGD06]. hexadiyne [PA05]. hexadiyne [PFWS01]. hexagonal [BK08, LTF07]. Hexahelicene
hydration-parametrized [RSP03]. hydrazines [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JJIH01, LLXS02]. hydrides [KS01b, SSB06, dSGDG06]. hydridotris [HT05]. hydrindans [HKHN08]. hydrazine [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JJIH01, LLXS02]. hydrides [KS01b, SSB06, dSGDG00]. hydridotris [HT05]. hydrindans [HKHN08]. hydrocarbon [CS01, KFD06, LC06, Wan09, WEE01]. hydrocarbons [Bor03, BS03, EB04, FVB08, LS08c, MGGM07a, SDvG01, VS08, WFHP01, WJ00, ZKZ07]. Hydrodynamic [BZP09]. Hydrogen [AG00, Kle03, RP04, XZ04, ZX04, AD00, AST06, BM07, BUMCMRL00, BL06, CUS00, CUS03, CPDZH08, CVVB04, CCK01, CDPL09, DR07, EFQD09, GAIMVB01, HIdMS05, HIdS06, HRG07, HIA03, HT03, HA04, IO08, JP09, mJIZsLyL07, Kle02, LC07, LDC+07, LW04a, LDL+09, Mck07a, MH08a, NNH05, OO08, PG01, Pac06, PGG06, Pog06, Rao00a, RM07, SPT+03, SJW09, TGLL07, WLLS04, WZZ09, Wi01a, WLL+03, XLL+02, YTN1, ZSC05, ZW09, ZGZX07, ZG09, vEMK01, vE01, Yos02]. Hydrogen-abstraction [WLLS04]. hydrogen-bond [RM07, SPT+03]. hydrogen-bonded [CPDZH08, LLD+09, MH08a, ZH08, vEMK01, vE01]. Hydrogen-bonding [AG00, ZW09, Yos02]. hydrogenase [TDH06]. hydrolases [OB09]. hydrolyses [DWS+09, LDL+09, MH08a, ZH08, vEMK01, vE01]. Hydrolysis [WOC+03, DLR+08, MBH+00, RP04, TH02, WJX+08]. hydroperoxy [BL06]. hydrophilicity [DLHC06]. Hydrophobic [MBH+02, CJDK09, HJCP01, SDL07]. hydroxide [CBS+03]. hydroxy [AZM03]. hydroxyacetone [WXX03]. hydroxylaromatic [BLO+02]. hydroxyformaldoxime [TT02]. hydroxyl [CUS00]. hydroxylase [HLC09]. hydroxymataresinol [SH09]. hydroxyproline [BISB02, PRK05]. hyper [Mar03, vGGB00]. hyperconjugation [CPDZH08]. hyperconjugative [BPC01]. Hyperpolarizabilities [MO01, CJK+02, LWZ09, Tor02]. hyperpolarizability [JPCA08, XWL+09]. hypersurface [SSBE06]. hypersurfaces [SPC+01]. hypochlorous [JKM08]. hypothetical [LD05a]. hypoxanthine [KKMMS04]. hypoxanthine-cytosine [KKMMS04]. I/O [SSL02]. ICFF [KTA03]. Icosahedral [EL07, LML+00, OSA06]. IDE [Gen09]. IDEA [DBGV07]. ideal [Pan07, STSF02]. ideal-gas [STSF02]. identical [CS05]. Identification [CP09, FWH+07, KS05b, PPXP01, SL+09]. identify [LHJ+06, ZS04]. Identifying [CCC09, DBH02, CLS+09, HL0+05]. identity [DSR+07, Nee03, RC04]. idiosyncratic [CMCB08]. II [ACM+06, DPT03, DF04, FNP+06, FK+09, GPK05, LPP06, NK06, Sha02, TGGP+00, WM01, BHW00, BA04b, Ber03, Car02, CSB08, EBD+01, EK02b, GGB07b, HZ06b, Ish03, JJB02, Kle03, LLA01a, LFZ04, LCA03, LMIF06, MB00, OBBS05, PMB04, PV03, Rld05b, TMJ+03, TC+02, WIP02, WNH03, WFR08, vEMK01]. III [BB08, DF04, FR05, KPR04, VHR07a, YIN03, CCB04, CG05, KEB04, LLA01b, LCA03, ZFL+05, vE01]. Illustration [KS02a]. image [IC08, XWC09]. IMiCMO [MS01]. imidazole [JKM08, PGG06]. imidazoline [XKG+05]. imide [CXZ+09]. imine
Bor03, GTC06. **Imipenem** [SDM02]. **Immune** [WCS09]. **Immunoglobulin** [Kr03]. **IMOMO** [VM00]. IMPACT [BBC+05]. Implementation [AKN07, CKW09, DRMD03, KBT03, LI07, PSZ04, RNG03, SVT09, YTH+07, BMRD01, BLMS08, DFWH05, DBS08, FROD08, GY06, JNV08, NBJ04, PZWG+04, SAM06, SM08b, TTO1, VK06, WCC08, YCXY03, LLL03, VW03, YOB+08]. implementations [FL08]. implemented [HP01, MP3b]. implementing [OR05]. Implications [AKN07, CKW09, DRMD03, KBT03, LI07, PZS04, RNG03, SVT09, YTH+07, BMRDB01, BLMS08, DFWH05, DBS08, FROD08, GY06, JNV08, NBJ04, PZWG+04, SAM06, SM08b, TTO1, VK06, WCC08, YCXY03, LLL03, VW03, YOB+08]. improvements [FL08]. implicit [BBHD04, BLL+06, GL04a, JS07a, JZZ+09, KTA03, Kro03, Lab08, LSO04, MCM04, PSZ04, PPYS08, SBK01, SL06, WL09a, ZGLF01]. Implicit [CGBF05, ENM+04, ZM06, HLC09, JW06, OCB02, PMPGP05, PPM05, TS05]. important [CSU05, EDAJ04, Tor02]. Improper [TNS00]. improve [FSM09, XLT07]. Improved [CN03, CLA+00, Gri03, HQQ2, KK08a, KK08b, LK04, RCJ02a, SKSH07, TGD05, Wil01a, Wil01b, CMBC08, DSR+07, KDSV02, MP03b, Maz08, MFR07, PABK03, PRS04, SDvG01, STSF02, SHK+05, VZM+08, LK03, RCJ02b]. Improvement [SM08b, UKN04, Nee03]. improves [CLWL09, RK05]. Improving [BUMCMRL00, Bie04b, GF08, LJ04, LKW04, GRO+03, GP06, SMG09]. in-core [FR06]. inactivation [PFR04a]. incidence [YWZH03]. Inc1 [ZL05]. Including [CQ08, AKN07, DP03, DP04, Gri04, Ish03, LB08, SL09, Wil01a]. Inclusion [HK08a, HK08b, PWHF+03, PWHF+04]. incomplete [FWH+07, Ish04]. incompressible [ZHWM09]. incorporate [KTA03]. Incorporating [CLS+09, DMJ05, HLT+05, SLC+09, HS01, LL07, RD06]. incorporation [SM06]. Increasing [ZWZ09, BT00, LJ05, YACL+02]. independent [FVBO8, OTL08, Van02a]. index [COH01, JLHF03, MBH+02, PVJBO0, Pog03, YWZH03, YW04, YW07]. indexing [HWDB03]. indicators [BWW+08, HIM07]. indices [BLT03, CGMPT+08, FZL07, FMPS08, FVB08, FS04, GDPCPU07, GMGM07a, GMGM07b, May07, Rao00a, SPGS08, TSMG01, TSSG08, WMW03, WW03, WMW04]. indium [ZL05]. individual [ZM06]. INDO [PBZ00, TY03]. INDO/SCI [TY03]. indole [LL01]. induced [CGB03, CMCB08, EDW07, HIM07, HHP04, KIFK07, LGB+09, LBG08, MLA00, PSF+08, RSN+02, ST01, ZALMG03]. Induction [HK08c, HK08d, ZOJ+06]. Inductive [BE07]. inelastic [BACJCT01]. inexact [Har04]. inexpensive [KFZ03]. infinite [DA01]. Influence [GSB09, JS07a, JT08, LZA02, BGC+09, SBH02, SLRC01, DB06, EL09]. Information [Ham07, GCB03, HTKG08, HP05, NL08]. information-bearing [NL08]. infrared [CVR08, Kle03, LDL+09, MGLDS00, TDH06, Zer08]. Inherent [BYQS03]. inhibition [PFR04b, WC08]. Inhibitor [VVS07, BMTFR08, CVW+05, FPG+06, MBC08, SVV+08]. inhibitors [AJNG01, AGO+02, APG05, AVS09, LLL+08, LZ05b, PB06, RGP+07, VB09, VVS07, WZY04, WHF08, ZWB09]. inhibitory [DD08]. inhomogeneous [MFL08]. initial [MM03, MABM09, Qua07, UNM+01]. initialization
initiated [RAGLL09b]. initiation [GGGLL05]. initio
[AJ03, Ama02a, Ama02b, Ano06b, ASY01, BG03, BG00, BL08, BSB05, BS01, BL06, BLO+02, BSJ01, BZL05, CPJ00, CPM03, CUS00, CU01, CUS03, CLO9, CYM02, CJW+09, CHRL09, DGD+05, DWS+09, DPM09, DB06, Dra00, EM03b, FG02, FAR02, FO08, FNP+06, FKU+05, FKM+06, FKS+09, GKRG08, GD06, GBB07, GGLR00, GKTS04, GPK05, GBBH09, Haf08, HS07a, HTSR04, HSWW00, HJCP01, ITS05, ITS06, JCA+02, JFG04, JCHS07, KSB+02, KP05, KFNH08, KKG+09, Kiel02, KF02a, KIFK07, KWK+00, KPR04, Kri08, Kri09b, LMK01, LYK+04, LDC07, LMCD09, LMB08, LZJ03, LWLS07, LKT04, LF02, LXS08, LLL07, LZF+09, LMO09, Mar03, Mas01a, Mas01b, MDA08, MGLD00, MLL08b, MM02, MS00, MIA09, MG00, MLD01, MW00]. initio [MS01, Mor02, ML00, Mii05, NYK+09, OO04, OON01, OS08, ON07, Oo08, PP08a, PGN03, PGRRNG03, PHRR08, RSSKB03, RSE07, RRCA08, ROG00, RGG08, SS00, SG07a, SAS05, SBL05, Sha02, SLL+04a, SSS+09, SRE08, SMK00, SMZW05, SK05, SSBE06, TASS07, TYN05, TZX01b, TZX01a, TGGP+00, TFZRG01, UCT+03, UM03, UTM+02, VSK+04, VS02, VIP+06, WKG07, WLL07a, WS05b, WOC+03, WDX+02, WXX03, WCL05, XLL+09, ZE08, ZZZ04, ZZZ+06, ZW09, ZGX06, ZX08, ZWT0+08, ZL90b, vDSSvA04, vEMK01, vE01, CSV+07, MD04, SH07, TB00]. inner
[Pog03]. inner-core [Pog03]. inorganic [CMA+08, SYY+03]. inserted [BL08]. Insertion [ZSVSC08, RD00, TB00]. insight [MDA08]. Insights [BTP09, PSHP08, SBG+09a, MCK05, PAS07, SGS03]. instabilities [DD00, vW06]. instability [LPK07]. instead [Lab08]. insulator [RDM+08]. insulin [ITN+05, KVS+06, ZM06]. insulin-B [KVS+06]. Integral [JCA+02, BR00, BR01, CC09, CJ09, CF04, DBS08, GMW08, JP09, KJVW08, Lab08, MBWP03, SVT09, UK04, Vya01, Yas08, PVdJB00]. integral-driven [SVT09]. integrals
[ABF+03, FL08, FMAMRK06, FR06, GA00, Ish03, Lai07, RL04a]. integrands [GC03]. integrate [MP03a]. Integrated [BBC+05, HT03, LOL+08, MS01, VKCK09, VM00]. integration [BK00, Bli04, CLF+09, ESP04, HW03, JCA+02, KBA+04, LRW03, Pom04, RP07b, SY09]. integrations [PF05]. integrator [CF06, KMO0, QNF09]. intensities [WKYU01]. Intensity [Tor02]. Intensity-carrying [Tor02]. Inter [HRBB03, MAF+07, RP02, SWV+05]. Inter- [HRBB03, RP02, SWV+05]. inter-phycoerythrin [MAF+07]. interacting [RG08, YCXY03]. Interaction [BE09, GBBH09, LSAS01, MHS05, ROG00, AKN07, AB04, AZM03, BRLS08, BRLS12, CLC09, CF04, CF+08, CPML08a, DLD+02, DMZT08, FQ07a, FL07, GD03, GMW+00, GS04, GKT04, HZ06a, IDMC09, Ish03, KN04, KBT03, KS05c, LDMR01, LWX07, LP03, ML06, MN02, Mas04, NTH09, OS09, PP0P01, PMPG05, PRSM02, PRSMA08, RRCA08, SKG00, SSL02, SYC03, SWZ04, SLRC01, TZH03, UT0+02, VC04, WS05b, ZC03, ZWP08, EB04, JCHS07, LFZ04].
Interactions [CPML08b, FKŠ+09, Van08, ALC08, AG00, ASDP+06, ATMK03, Ano05b, AS00, BPC01, BM07, BUMCMRL00, BSJ01, CMaGL+04, CEP07, DDBP09, EFQD09, FÁ01a, FO08, FNP+06, FKM+06, FKM+07, GGP09, Gon07, HLC09, HA04, HZ06a, HZ06b, IINK09, IB04, JWB05, KF02b, KH06, LHI+06, LCC09, LZJ03, LS08c, MM05, MMLC05, MCF07, NK06, Nil09, PG01, PCO+07b, PCO+07a, PK05, PNG08, RZWS07, SOOF05, San01, Sha05, SS+09, SWV+05, SG01, SL06, SDL07, SMV+09, UTT+04, VW03, WR+06, WPH+07, Won09, YT03, YTH+07, ZTS09]. interactive [DFGB09]. interactively [SB01]. Interatomic [RD06, AMR04, SS00, SPT07]. interconnected [SB08]. Interconversion [OO04]. interconversions [FD03]. Interesting [Kri09a]. Interface [CW02, DPDG05, FOK+04, GKRG08, HHBH00, HZX04, JKII08, KKG+09, LLL03, LPB03, PHJ+08, SWM04, TDMSD+08, ZCS04, DBGV07]. interfaced [FKL+06]. interfaces [BSH07, ZZTS09]. interfacial [CW02, MWL+08, PHJ+08]. Interfacing [WHG+07]. interior [SYC08]. interlayer [ALC08]. interlayers [DJT08]. intermediates [BLO+02, BMTFR08, IGNH03, MMMY07, OBT09, WSM+09]. Intermolecular [PSC+01, AS00, CMaGL+04, CLC09, FÁ01a, FKM+06, FKM+07, GGP09, GS04, IGL07, KS05c, LZJ03, Mas04, PMPGP05, RRLA08, SPDS01, SJW09, UTM+02, UTT+04, Wi01a, Wi01b, ZDS+05]. Internal [EA06, BHH+09, CFD03, CFD04, COMR+04, DHE+05, Din00, HFS003, KSD03, KTA03, LPK07, SWM04, TDM+08, ZCS04, DBGV07]. internal-rotation [DHF+05]. interpolated [YK08]. interpolation [BB05, IS03]. interpretation [CPJ00, HLS07, VM07]. intersection [SSHT03]. intersections [IK00]. interval [LS05a]. interwall [ZZvRSC08]. Intra [FÁ01a, FKM+06, FKM+07, MAF+07]. Intra- [FÁ01a, FKM+06, FKM+07]. intra-phycocyanin [MAF+07]. Intramolecular [GKTS04, HA04, PG01, TFZR01, AGK03, BA03, BA04a, FDA00, HRB03, HK08a, L01, NH01, RP02, SWV+05, VIP+06, ZDS+05, ZW09, ZH08, Kle02]. Intraprotein [MLJ03]. intraresidue [IB04]. intrinsic [JS07b, JT08, YGZZ05]. intrinsically [NAT07]. Intruder [CWY09, WCFH02]. intuitive [PP08b]. invariant [Est07, ZLY07]. Inverse [BR03, MLL08a, Nil09]. inversion [KSTC01, RC04, ZSE08]. investigate [DWN01]. investigated [HN02, Kle03, YH09]. Investigation [LZLC09, YTH01, AST06, BLO00, CW02, CHA+07, CG08, GS03, GS04, Hir08, JH01, KYFW07, LH02, LXS08, NS08, PV07, QZZZ03, QZL+04, RM07, RC04, RV09, SL04, TGQ+00, TFZR01, UCT+03, WL09b, WL+07, ZXY08, ZKZ+07, ZHWM09, ZGXX07, JB03, JBG08]. Investigations [JP09, WGO2]. involvement [BLO+02]. involving [LL01, MM05, ZGXX07]. iodides [CM09]. iodine [GWM+00]. iodobenzoylphosphonate [GWM+00]. Ion [DAK08, BM08, Dra00, EL07, FHR07, FL07, GWM08, Gor01, IsV06, KPR04, Kri08, Kri09b, MSBS01, PPYS08, PHRR08, RC04, VHR07a, VHR07b, ZZW09, dOMSL01]. ion-pair [RC04]. ionic [Ang09,
ionizable [OS06]. ionization [GSB09, KFD06, RTG00, SVT09].
ionospheric [LSHR04].
ionization [GSB09, KFD06, RTG00, SVT09].
ionospheric [LSHR04].
ionization [GSB09, KFD06, RTG00, SVT09].
iron-containing [MHS05, RMP01, SL09, ZSC05, ZZZ+06]. IR [GZ07].
iron [GZ07]. IR [NRKH02, ZWTP+08]. iron [DPT03, GK09, HLLN06, LWH06, MHS+06b, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06].
iron-containing [MHS+06b]. regular [ZBS03]. irrelevance [VVBV02].
iso-energy [Rap06]. Iso-guanine [GWL07]. isobaric [SM03, Ste04].
isocyanates [OY01]. isocyanide [HT05].
isocyanurates [OY01]. isoelectronic [Che01]. isolated [RZWS07]. isomer [HLLN06]. isospecific [AGK03, GVATG03, RGP+07]. isomorphic [CRGN07].
Isomers [Ber03, CCB04, GB02, CDL06, CTFC08, HYA02, KYFW07, KZY09, LS08a, LMO09, Sau04, ZZZ+06, ZZvRSC08]. isomorphic [CRGN07]. isospecific [CRGN07].
isotopes [GWM08, WDX+02, GM04]. isotopologues [LMB08]. isotropic [BCIB05].
isozymes [WC09]. issues [Mac04, PHFC04]. Iterative [PU09, Rao00b, CC09, HZ06a, HZ06b]. itinerant [SM08a]. IV [AZM03, CN05, CDL06, DMIN05, FZL+06, LLA01c, LLA03, LCA03].

J [BPC01, Bof01, HNW12, Kne05, Qua01, Van08]. Jacob [IR03].
Jones [CYM02, FSFK05, Pul05, SCC04, SYC08, YCS07]. Journal [Ano05b, Ano06a, Ano06b, Ano06c, WB04a, WWC+05, Ano01c, Ano04b].
journey [PCD+09]. jun [KK01a]. junction [DWN01]. Junmei [WWC+05].

K151 [NYK+09]. Kenny [Sta00]. Kepert [RMP01]. kernel [BR00, BRS01, DDV09, TSSG07, TSSG08]. kernel-based [DDV09].
etene [MGG06]. ketones [LLA01a]. key [HEP+02]. Kick [AM09]. Kier [SPGS08]. Kier-Hall [SPGS08]. kinase [FCP+04a, FCP+05, GdSuM+07, HLT+05, HW09, KKO1a, PB06, SWV+05].
kine-channel-phosphatase [FCP+05]. kinase-specific [HLT+05].
kineses [SWM04]. kind [LX07]. kinematic [CSJD04]. kinematics [CCC03, LFKL00, LLL08a]. kinematics-based [LFKL00]. Kinetic [mJZL07, Bie04b, BZL05, GWM08, Jac09, Kri09a, WDX+02]. Kinetics [CUS00, ST04, Gog08, HLS05, MG06, NSU+02, MLB08, UNM+01, VW00, VW04]. kinking [BCP03]. Kirchhoff [YOB+08]. Kirkwood [KS06].
Kirkwood-Buff [KS06]. Kneller [CSD05]. knowledge [Adc04, HZ06a, HZ06b, LWV+06, NMAT01, dSR08]. knowledge-based [Adc04, HZ06a, HZ06b, NMAT01, dSR08]. Kohn [RRS07, Bou00, SH02]. Kollman [JVK09]. Kr [CMJ08, CGB03]. Kroll [YH09]. Krylov [Har04]. krypton [CVVB04].

L [Bac09, HT05, JPF+00, PC00, AGO+02, HT05, HJC01, KOML08, NYK+09, OYK+09]. L-2-haloacid [NYK+09]. L-captopril [AGO+02]. L-cerebroside [AGO+02]. L-cysteine [AGO+02]. L-cystine [AGO+02]. L-phenylalaninamide [HJCP01]. L-valinamide [HJCP01]. LADH [DMC05]. LaN [VP08]. Lanczos [MO01]. Landau [GHH07]. landscape [IGNH03, PAT+09, SPL+02]. landscapes [OKH+02, SSB07]. Langmuir [BRS00]. lanthanide [AB00, FRS05, RMP01, SNM+06, VMA03]. lanthanides [RD06]. Lanthanum [AB00]. Large [WCF04, ARL01, AB08, AS00, BG03, BP01, BdPRMAI00, BME05, CJK+02, CDD+02, CG06, DMN03, DJB02, Ell07, FZL07, HB09, HSM06, IME02, IS07, JO02, JW00, KS05b, KKG+09, KK01a, KH06, LJ02, MKGA06, MH09, MHW04, MH08b, MPF00, ME06, NRK02, PFJ+03, RRS07, SYC08, SSL02, TY0+02, VSK+04, WWL+09, YCS07, vGB00, WS07]. large-amplitude [KS05b]. Large-scale [WCF04, DMN03, JO02, KK01a, MH09, MHW04, MPF00, ME06, RRS07, SSL02, TY0+02]. larger [VKP+08]. lariat [ZWY+09]. laser [Sha02, KZW+05]. latency [KVF+07]. latter [LPK07]. Lattice [OGH05, SG01, HP01, KWK+01, KWK+02, KFO2b, LJK08, MH08a, SCC04, SYC08, TK08, VGDS08, YCS07, vE01]. law [Sch00]. LCAO [EBL+08, EL09]. LDA [RLD09]. lead [RS07a, RS07b]. leads [PPXP01]. learning [YCW+09]. least [CSD05, Gol09, LLZ09]. least-square [LLZ09]. LEDO [GKH05]. legacy [Sha07]. Lei [Ano06c]. length [CRC+08, DR09, JPCA08]. length-frequency [DR09]. lengths [PSC+01]. Lennard [CYM02, FSFK05, PUL05, SCC04, SYC08, YCS07]. Lennard-Jones [CYM02, FSFK05, PUL05, SCC04, SYC08, YCS07]. lesion [Pin01, SHD+08]. lesioned [Pin01, Pin03]. Letter [BFS07]. Letters [JW12, WM12, vLBBR12]. level [BUMCMRL00, BLT03, BL00, DPM09, JMD+02, mJlZsLyL07, KK08c, PFJ+03, RC04, TAB00, PST+08, UTM+02, WyL+09, WS05b, WLL+08, ZOL+05]. levels [BACJCT01, CUL04, DJB02, PFJ+03, WW03]. Lewis [BHTCG07, GR07, Sha07, Sim07]. LF [PWHF+03, PWHF+04]. Li [CRC+08, GBDP05, JW12, HDO+02, LWKO8, LW+06, LAT05, WWT08]. libraries [AL01, KV00, LZ05b, ZM09]. library [CRH+07, FAB+00, KSM05, OTL08, SH07]. LiF [EL09, UM03]. lifetime [CHA+07]. Ligand [MKT04, AM06b, BPS06b, BGC+09, BS08, BMTSC01, CGB+09, CLH+07, CN05, DFWH05, FOU8, GZM09, HZ06a, HZ06b, HW09, JZD+09, KS08, LW+09, Mue01, NR04, NMAT01, OFIK09, PWHF+03, PWHF+04, RK05, Ruv07, SOOF05, STSF02, TFN04, TJE03, VGGMM05, VOG05].
XZZ04, YK00, Yan04, ZGFL01, ZWS+02, BDW00, HLC09. ligand-charge [BSP06b]. ligand-protein [VGGMM05]. ligands [BS05, CKMC04, FO08, FUK+05, GTC06, GM01, GGLR00, JFG04, RGG08, SWM04, TP01a, TGGP+00, WS02b]. ligation [KT08]. light [KrÓ3, LFR07]. light-emitting [LFR07]. lignin [PS09b]. LiH [McD03]. like [BCIB05, DHW00, DBI02, FZL+06, JD09, Kut07, LAEL01, PRKP05, WL09b]. limit [MV06, MLL+08b, PSC+01, SAS05, Var09]. limitations [BYQS03, LFEdL06, PRDS08, MFB04]. limited [Ano05b, Sha05]. Limits [OV03]. line [RHL09]. Linear [Con02, DLWV07, KDG+09, LMJ02, OS06, OFIK09, SKDO08, vDVGD00, AT02, ABA04, BH03, BPCD07, CC09, CGMPT+08, GCDL+05, Gol09, GGLR00, Har04, KLM+09, MW09, McD08, Oos09, PK05, RI07, RS05, SSB+03, TCR+02, vGGB00]. Linear-scaling [OS06, SKDO08, GGLR00, TCR+02]. linearized [ABWT09]. link [GdAcV+07, KS02b]. linkages [SDL+09]. linked [CMD+04, CHRL09, FS98, FS00a]. LiPF [BSJ01]. lipid [HN08, RGG08, SSM08, WC09]. Lipkowitz [Sta00]. lipophilicity [DMC05, DLHC06, DLHC06]. lipoxygenase [TGLL07]. lipoxygenase-1 [TGLL07]. LiPt [LWK08]. liquid [BM08, CC07, EGSG00, GDV03, GJK00, HPL03, MM07, NL07, PHJ+08, PB04, POJ01, YGLvG06]. liquid-state [POJ01]. liquids [CF04]. list [PABK03]. lists [KUB07]. lithium [HXD08, LWLS07, RC04, SLRC01, YSA+03]. liver [CMCB08]. LMO [BY06]. Local [Diu00, LYS08, AGSFAL05, CPML08a, Ion07, IS03, JHPRSM+05, KMA+07, LMJ02, MA09, PMC+08, RUPH06, SL09, SEKS09, SB08, TT05, TSSSG08, VKCK09]. localizability [BK08, BW+08]. Localization [Che01, ALT06, FS02, FSS00, GB03, P08b, PA05, PAS07, PC05, PC07, SFC04, ST01, WMW03, WW03, WMW04, SHBD05]. Localized [ABF+03, AB09, Bac04, Bac05, Bac07, BME05, FMSA06, GFS05, ITN+05, TT01]. locally [TY0+02]. locate [ABB01a, ABC01b, Bo01, GMA04, MP03b, Qua01]. locating [WSM+09]. Log [Tot04]. London [Lab08]. Long [RP07c, CCSJ00, CPC+00, CE07, CSRST04, Gr06, KSS08, LYS08, MN02, MBC08, RLP08, San01, VVB02]. long-duration [CCSJ00]. long-range [CE07, Gr06, KSS08, MN02, RLP08, San01]. long-time [CPC+00]. lookup [Nil09]. loop [CSJD04, KK01a, Mak08, OFB08, RPT+07, RPT+08, TLKT00]. loops [CSRST04]. LoProp [SKK+07]. Low [DPT03, MG06, AG00, BS05, GS03, KUB07, KK01a, KK01b, LAS+03, LB08, LBP07, OFJ+03, PRSMV08, Rao00b, Sha02, WS02b, ZL05, ZL07, ZL09b, dSV+09, BS08]. Low- [DPT03]. low-energy [Rao00b]. low-level [PFJ+03]. low-lying [LB08, ZL05, ZL07, ZL09b, dSV+09]. low-mode [KK01a]. low-resolution [BS05, WS02b, BS08]. lowest [FD3A00, OA06, ZJ04, ZJ04]. lowest-lying [FD3A00]. ip [LAR+03]. ip-RS-HDMR [LAR+03]. LR [ZWB09, NSF+07]. LR-MMPBSA [ZWB09]. LSCF [FAR02]. Lu [SNM+06]. lumiflavin [CNN07]. LUMMOX [MS04]. lutetium [AB00]. lyase [PMM05, CJPZS08]. lying [FD3A00, LB08, PRSMV08, ZL05, ZL07, ZL09b, dSV+09]. LYP
Lysine [DJT08]. lysozyme [HN02].
[GMA04, HFSD03, LHI09, MMLC05, NMAT01, RNG03, YCXY03]. **mean-field** [KRM+02]. **meaningful** [AE06, Bud07]. **means** [Bac05, Bie04b, BLF02, Kar06, KBL08, SMAdV00, WKYU01, DOMSL01]. **measure** [XSHC06, ZHH09, PDC+08]. **measurement** [YZ04]. **measures** [KBLO09]. **measures** [BDW00, DW08, Ham07, LeH06, PYEA03, PCA+08, PDC+08]. **mechanical** [AVB00, BISB02, CLP09, CGBF05, CCK01, COL+06, DWC+03, ECA06, ESM06, EBD+01, FHRR07, FA01a, FAB+00, FAM01, GAILVB01, GGLR00, JHH01, KK03a, MBL+00, SA04, TCR+02, VHRR07a, VHRR07b, XZZ04, XLZ08, YPNE09, ZC03, ZAT07]. **mechanical/molecular** [CGBF05, FA01a, TCR+02, VHRR07a, VHRR07b, XLZ08, ZAT07]. **mechanics** [AS06, AS09, AD00, AM06b, AG01a, APA05, BDW00, CLFA07, CR02, CSU05, DPT03, DFWH05, DWC+03, EC06, FEVM01, GCD+08, GS04, GKS04, GPK05, HWT03, JCHS07, KLB03, KZ003, LL00, LL01a, LL01b, LL01c, LL01d, LL03, LS08, MLA00, MF04, MPF00, OSH03, PRK05, PS09b, PWPH+03, PWPH+04, RMP01, RSE07, RP02, ROG00, RM00, RGB+07, SS00, SHD+08, TGGP+00, TFZRG01, TT05, VSW+00, YSA+03, ZSK07]. **mechanics-based** [BDW00, RSE07]. **mechanics/molecular** [MPF00]. **Mechanism** [AS06, AS09, AD00, AM06b, AG01a, APA05, BDW00, CLFA07, CR02, CSU05, DPT03, DFWH05, DWC+03, EC06, FEVM01, GCD+08, GS04, GKS04, GPK05, HWT03, JCHS07, KLB03, KZ003, LL00, LL01a, LL01b, LL01c, LL01d, LL03, LS08, MLA00, MF04, MPF00, OSH03, PRK05, PS09b, PWPH+03, PWPH+04, RMP01, RSE07, RP02, ROG00, RM00, RGB+07, SS00, SHD+08, TGGP+00, TFZRG01, TT05, VSW+00, YSA+03, ZSK07]. **mechanism-based** [PFR04b]. **mechanisms** [AG01a, AGI+07, BS06, CCCJ09, CG05, ILKR09, KZ009, KKH09, LLK06, MK02, NS08, RO04, SIO04, TMBM02]. **Mechanistic** [BMTFR08, SGS03, TT02, AN06a, ST06, WDS06, XDS06a, ZLS06a]. **media** [HLN06, MM02, SM00]. **mediated** [HIA03]. **medium** [FZL+06, HXL09, LF04, LFZ04, SH07, ZFL+05]. **medium-resolution** [HXL09]. **medium-sized** [SH07]. **melatonin** [KT+08]. **mellitus** [PS09a]. **Melting** [LML+00, KT02]. **membered** [FJ08, ZW09]. **membrane** [ALB09, CJ09, DA08, FC04a, GAS04, ILKR09, JM07a, LB03, MHJ06]. **membranes** [Ike01, SSM08, W09]. **memoriam** [AN00]. **memories** [WHRG08]. **memory** [TY02]. **mercaptocarboxamides** [TFZRG01]. **mercaptocarboxylate** [AP05]. **mercaptopyridine** [YXZ+04]. **mercury** [FNP+06]. **Merging** [JPJDPRM07]. **Merz** [JY09]. **Merz-Kollman-Singh** [JY09]. **mesh** [BYQ09, KM00, KSY+00]. **mesoscale** [RPMP03]. **Mesoscopic** [YPNE09]. **Met-enkephalin** [ZCL09]. **meta** [DDBP09, ION07, ZTP+08, GA09]. **meta-di-fluorobenzene** [ZTP+08]. **meta-generalized** [ION07]. **metabolites** [PCMG09]. **metabolizing** [VB09].
metabotropic [FTLV01]. metadynamics [BBP09]. Metal
[SGD06, ABYM08, Ano06a, Bac05, BTP09, BS06, BRV+07, BM00, BWI+02,  
CM09, CZX+09, CWWS07, DSB+02, Dra00, FO08, FKRE08, GM01, GS04,  
HZX04, Ho05, HSWW00, IC08, JHMB+09, JHMB+11, JKL08, KT08,  
KRM+02, KEM08, LW07, LML+00, LWK08, LMGR06, LS02, LWZ09,  
MSBS01, NR04, PYCD03, PLC08, RRFC+03, SL09, SZTO8, ST06, TAS07,  
VHR07b, WB07, WWT08, Wa06, YTH01, ZSC05, ZYW+09, ZX08].
metal-catalyzed [HSWW00]. metal-free [CM09]. metal-organic [TAS07].
metal-porphyrins [SGD06, ABYM08, Ano06a, Bac05, BTP09, BS06, BWI  
+02, CM09, CXZ04, DSB+02, Dra00, FO08, FKRE08, GM01, GS04,  
HZX04, Ho05, HSWW00, IC08, JHMB+09, JHMB+11, JKL08, KT08,  
KRM+02, KEM08, LW07, LML+00, LWK08, LMGR06, LS02, LWZ09,  
MSBS01, NR04, PYCD03, PLC08, RRFC+03, SL09, SZTO8, ST06, TAS07,  
VHR07b, WB07, WWT08, Wa06, YTH01, ZSC05, ZYW+09, ZX08].
metal-porphyrins [SGD06, ABYM08, Ano06a, Bac05, BTP09, BS06, BWI  
+02, CM09, CXZ04, DSB+02, Dra00, FO08, FKRE08, GM01, GS04,  
HZX04, Ho05, HSWW00, IC08, JHMB+09, JHMB+11, JKL08, KT08,  
KRM+02, KEM08, LW07, LML+00, LWK08, LMGR06, LS02, LWZ09,  
MSBS01, NR04, PYCD03, PLC08, RRFC+03, SL09, SZTO8, ST06, TAS07,  
VHR07b, WB07, WWT08, Wa06, YTH01, ZSC05, ZYW+09, ZX08].
metal-organic [TAS07]. metal-porphyrins [SGD06, ABYM08, Ano06a, Bac05, BTP09, BS06, BWI  
+02, CM09, CXZ04, DSB+02, Dra00, FO08, FKRE08, GM01, GS04,  
HZX04, Ho05, HSWW00, IC08, JHMB+09, JHMB+11, JKL08, KT08,  
KRM+02, KEM08, LW07, LML+00, LWK08, LMGR06, LS02, LWZ09,  
MSBS01, NR04, PYCD03, PLC08, RRFC+03, SL09, SZTO8, ST06, TAS07,  
VHR07b, WB07, WWT08, Wa06, YTH01, ZSC05, ZYW+09, ZX08].
metal-organic [TAS07].
methoxycarbonyl [KK09]. Methyl [CADW03, CCK01, DBM03, DMR05, HT05, RC04, WLX05, WDS07, WSM08, WLL03, WC08, ZLS05].
methylacetamide [MMPK01]. methylacetylene [ZKZ07].
methylamine [LMB08]. methylation [EL07, HM08, SCL09].
methylene [LFS07]. methylenimine [dOMSL01]. methylenimmonium [dOMSL01].
methylimidazole [HT05]. methyloxaziridine [ZPL07]. methyloxirane [ZPL07].
methyltransferase [WC08]. MF [DHW08]. MF-3D-QSAR [DHW08].
Mg [WZZ09, AS06, LST08, SBL05]. Mg-porphin [SBL05].
mGluR1 [FTLV01]. MgO [SBG09a]. MHz [CMD04]. MICCs [YGZZ05].
micelles [KS02a]. Michael [Ano00]. microcanonical [Rap06].
Microiterations [VMF03]. microscopic [PK04]. microsecond [MST08].
microsolvation [UM03]. microwave [ZGXX06]. middle [RPNJ07].
migration [HLB09, ZGZX07]. MILCH [BL09]. mimic [WMS06]. minima [CA04, DLL02, KG02, XOW00].
Minimal [BWZ09, BVW04, Maz01]. minimization [EGSG00, OM04, Sen06, WG02, vEMK01, ABF03, NCO05].
minimizations [dSR08]. minimized [GLD08]. Minimum [AM06b, AJO3, CZB07, CY09, CY13, SBL01].
minor [BCP03]. misfolded [CP08, WS07]. mispairs [SG07a]. mixed [FÁ01a, HELM09, MF00, MC06].
mixed-valence [HELM09]. mixing [AMR04]. mixture [WG02]. mixtures [FBDG06, NL07, YGLvG06]. MLR [HSMT04, LLL08].
MM [CGBF05, MF00, AST06, CR09b, CG05, FAR02, FMSA06, FSFK05, GWM08, GC04, GWM00, HHHB00, HBM06, HNR08, HRR05, HTNO3, IV04, lvSV06, ITS05, ITS06, KHF09, KPR04, Kri08, Kri09b, LLL03, MBB00, MK02, MSH06a, MG00, MLJ03, NGTB03, PB06, RG02, SBG09a, SN06, SMM08, SVV08, THIN01, TdMD08, VMF03, WCC08, WHF08, WHG07, WC08, YZ06, ZW09]. MM-PB [GC04, WHF08]. MM-PBSA [PB06]. MM2 [KKY01]. MM3 [AD00, LSWB00, YSA03, FH01, St05, SBH02, TAS07]. MM3/MM4 [AD09].
MM4 [AD00, CLFA07, LLA01d, LLA03, ACLD03]. MMPBSA [ZWB09]. MMVB [GRO03]. Mn [AZM03, BL00, GD06, BL00, PY05].
MND0 [DC02, RC02b, TBGRJ04]. MNDOC [IK00]. Mo [LZZC09, ML00, DRAS04, DRAS05, LDMR01]. MO/statistical [ML00].
mobility [HIM07]. MoCalc [DPDG05]. Modal [ES00]. mode [EBAN07, HRN08, KU03, JKP07, KKO1a, SFRS01, TVL03].
mode-specific [SFRS01]. Model [CPML08b, Duk01, EL07, Van08, AB08, ABBC01a, ABBC01b, AT07, APG05, BG00, BBHD04, BLL06, BT00, BCIB05, BB08, BLN01, Bo01, BLMS08, CFK08, CF04, CFC08, CP08, CP09, CRSB03, COMR04, CMGDAC07, CA07b, COL01, COL06, DLWV07, DHW00, DAK08, EA08, EDW07, EKO01, FKL06, FCK08, FEVM01, FC06, FBL08, FZL06, FNP06, GZL02, GL04a, GKO9, GJK00, GKTS04, GGT08, GWS02, HB09, HPL03, HS01, HK08c, HK08d, HHP04].
ILB03, JBB00, JJB02, JPF+00, JBGK08, KSB+02, KFZ03, Lab08, LRI+02, LAR+03, LFZSO4, LJ04, LSRR04, LR06, LK03, LK04, LKA01, MLW+08, MPPK01, MBOC08, Nak07, NL07, OKE+02, PCO+07b, PCO+07a, PMB04, PFC03, Pom04, Qua01, RPM01, Sen06, TJE03, TCT03, TGGP+00, Tot04, TV00, VW04, VGSU08, VP09, WCK00, WKYU01. model [WS05b, WEE01, WOC+03, WJX08, XL02, XZ05, XLT07, YL09, YPNE09, YJF06, vDSSvA04, FCP04b]. modeled [PB05, vDSSvA04].

Modeling [ECM+03, FRS05, MCR08, Mck07a, Mck07b, MTB09, PSCD09, SEKS09, Sie01, BA03, BA04a, NZ09, BSH07, CLP09, CJPZS08, DJT08, DMM05, EADJ04, ENM+04, GL04a, Gor01, HBM06, HMSM06, HMMS09, HRBB03, HP04, Hin00, JM07b, JTR05, KCL06, KS01a, KJP+07, KVS06, KPKZK06, LEK07, LLL+08, LFR04, MMLC05, MBM+00, MPF00, OFB08, SPGS08, SGS03, SYL+03, SSS07, ST05, TBB09, VBG+00, XL08, YKK09, ZBS03, ZMH+09, BBC+05]. modelling [PSHP08].

Models [JB04, AS09, AHGK09, ACM+06, CCK01, CPUGD09, CR07, CA04, CA07a, CEE+03, DNM03, DLG00, DR07, DDVD09, EC06, FHW+07, FK07b, GSB09, GDV03, GS02, GDPCPU07, GDPP08, GS08, HDM05, HD06, HP01, HLT+05, HG08, HIWC01, JPF+00, KOS02a, Kr03, JK00, LSL07, LSL08, LS08b, LT07, MTE04, MA05, MC06, OGH05, OYH05, PFD+03, PA05, QSS01, RD06, RSD03, RES09, RS08, RR05, SBLK01, Sch00, SS09, SRS02, SKK+07, SB01, SL06, VBS09, WB04a, WB04b, WB05, WZ07, YCBM00, YGLvG06, YJF06, YKK09, ZLC03, ZCL09, ZGFL01, ZLD09, ZWP08, TD06]. Modern [PB02, FLK07, Pra01]. modes [Gra07, LSY02, MGLL03, OR05, Tor02]. Modification [HN08, Vya01, YWH04, CM09, KFZ03]. Modified [LC06, NTH09, RC04, AVS09, CLA+00, KKY01, NA06, VVS07, WVS09].


[AS09, BBG+04, BG07, DWB00, CLC09, CLFA07, CCK01, DJT08, EMP07, FEV01, FPN+05, GJX00, HL09, Ish03, JTR05, KS05, KAS+07, KL03, KIM+09, LAA01a, LAA01b, LLA01c, LLA01d, LLA03, LSBW00, MLA00, Maz01, MO09, MS00, MST+08, NB04, Pin01, RPM01, RRZ08, SD02, VSW+03, WEE01, YSA+03, YGLV06, YK09, ZC03, ZWS+09, AM09, ARL01, AS06, AG00, ALB09, AD00, AGMPR08, ATMK03, AM06b, AB09, AGO+02, AP05, AS00, BG03, BP00, BR07, BA08, BB05, BWE05, BRDC02, BWZ08, BVW04, BT00, BS06, BME05, BS01, BPCD07, CM08, CO07, CDS09, CCL06, COS01, CW02, CI05, CDD+02, CK08, CSM00, CGB05, CF06, CO04, CPC+00, CR02, CCP07, CMD+04, CS05, CBH+03, DvG00, DB07, DPT03, DFWH05, DFGB09, DP09].

molecular [DSS03, DMC05, DLHC06, DK01, DWC+03, ESM06, EK02a, EK02b, FSM09, FHR07, FG02, FOK+04, FKL+06, FII+07, FA01a, FBD06, FLOD07, FAB+00, FKZ09, FEV+09, FKRE08, FNP+06, FRLN09, FUK+05, FKM+06, FKM+07, GL04a, GL08, GKR08, GCCV00,
multipole-based [WL09a]. multipoles [KS01a, SKK+07].
multipopulation [HIJ03]. Multireference
[WNH03, CWY09, DLD+02, HELM09, KBT03, MLL06, ME06, QTdG+08,
UKNS01, UKN04, WCFH02, dSVA+09]. multireference-MP2 [ME06].
Multiscale [San01, OFB08]. multiscaling [VTT+08]. Multispecies
[GDPP08]. Multistate [JHPRSM+05, FSM09, MST+08, YFS07].
multithermal [OO06]. mutants [GDPCPU07, MRS+07]. mutant [DLRZ09].
mutagenesis [MFR07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
mutase [HHBH00]. mutations [HFS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
multithermal [OO06]. mutagenesis [MFR07]. mutant [DLRZ09].
mutant [GDPCPU07, MRS+07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07].
NPT [Ike04]. NQR [MH08a]. NR [CPJ00]. ns [CMD+04, SO07]. NSAIDs [CMBC08]. Nt [ZNLL07]. nuclear [CR09a, CDL06, GM04, HWFN01, IKN08, QCK01, QCK02, WZXY07, ZPL07, ZXY08]. nuclearity [BACJCT01]. nucleation [CKW09]. nuclei [CDPL09]. nucleic [CCK01, DP03, DP04, FZL07, FM00, HWTL03, JCL05, MB00, Nak07, OMNH08, PPYS08, RKH03, SYC03, SL04, SWR06, SHK+05]. nucleobases [FKS+09, SB08]. nucleophilic [BSB05, SSB07]. nucleoside [Wil01b]. nucleosides [SA07]. nucleosome [VTT+08]. nucleotide [Mak08, MSF+08]. nucleotides [XWXC08]. nucleus [FVB08, HdMdS05, HdS06, HD06, IKN08]. NUCS [SHSF05]. nudged [AJ03]. number [CDS09, HXD08, KZRO03, KZW+05, KH06, TGGP+00, WWL+09]. numbered [GYCZ04]. numbers [GdAcV+07]. numerical [DLW06, LXL07, MO01, QNF09, TT08, WL04, vW06, DB07, ESP04, FMAMVK06, IO08, WL00, YK08, WG02]. Numerov [Bie04a, Bie04b]. Numerov-type [Bie04a].

O [BL00, GCCVB00, GPSP06, HYR06, ITS06, mJlZyL+08, KGL07, LZZC09, LMO09, Mas01a, Mas01b, NA06, Owe05, PGN03, PGRNG03, UCT+03, XWXC08, YHD+06, ZJM+07, ZY01, ZZL04, ZZL+08, ZXY03, Bac09, CCCJ09, DRAS05, Dib05, HM08, HDO+02, IS03, LC07, LW04a, LS05b, MGLL03, NyHN06, NHH06, RAGL09a, RFSS06, SSL02, SRE08, YLW07, ZXY08]. O-methylation [HM08]. O3LYP [BP03]. OB [NA06]. object [CRH+07, FL08, MVL+05]. object-oriented [CRH+07, MVL+05]. objective [WG02]. objectives [STCJ08]. objects [RSN+02]. observables [MG06]. observations [FWH+07]. observed [VBS09]. obtain [BVW04]. obtained [HFS03, VC04, WMW03, WMW04, WHH+06]. obtaining [Bac04, YGZZ05, SK09]. occupied [HHW08]. occurring [CJW+09]. OCF [UTM+02, UTT+04]. OCHF [YLW+08]. OCI [HLLS05]. OCLO [WLZ+07]. OCO [VM07]. OCS [VSO2, ZGXX06]. octahedral [OSA06]. octan [BE07]. octan-1-yloxy [BE07]. octanol [COL01, CSB+03, GOL9, Tot04]. octanol/water [CSB+03, Tot04]. octet [GR07]. Odd [CC07, GYCZ04]. odd-numbered [GYCZ04]. off [HP01, LJKL08, XLT07]. off-lattice [HP01, LJKL08]. off-plane [XLT07]. OH [Dib05, Gog08, HTN03, IvSV06, LW04a, Mas01b, WLL07a, CU01, CUSS03, GAIMVB01, GCCVB00, GGGL05, HTN03, KZY09, Kle03, KBBP09, LC07, LWY+09, Mas01a, MGLL03, Mui05, RAGL09a, RAGL09b, SEKS09, UCT+03, WLLS04, WLL+07b, WyLG+09, YLW+08, YLWL09, ZXY+08]. OH-initiated [RAGL09b]. OH-rotamer [KBBP09]. OH-stretch [Kle03]. OH/Cl [YLW+08]. OHO [Wil01a]. OHS [JP09]. olefin [PHKG07, YXC+07]. olefins [AVB00]. oligomeric [EL07]. oligomers [BSG07, CSJ01, Der09, LFR07, SBB02, WCL05, ZOJ+06]. oligopeptides [MGJAARC00]. Oligovalent [KS02b]. OLYP [BP03]. on-the-fly [KMA+07]. On-the-path [CY09, CY13]. One [CR09a, BG03, Bac07, Bie04a,
GKRG08, KFD06, Kri09a, Lai07, LB05, ZWS+02. one- [Lai07].

**one-dimensional** [Bie04a]. **One-electron**
[CR09a, BG03, Bac07, GKRG08, KFD06, Kri09a, LB05]. one-step [Oos09].
ONIOM [BGC’99, MDA08, MC06, VMF+03, XKKL03].
**ONIOM-molecular** [MDA08]. ONO [FJ08]. onto [NK06]. OOPSE [MVL+05].
open [CSV+07, FS02, PRSM03, LLA01a]. **Open-chain** [LLA01a]. open-shell [FS02]. open-source [CSV+07]. opening [SRE08].

**OPEP** [ACD’03]. operating [DFWH05]. operation [PCA+08, SYC08].
operators [KRM+02, Qua04]. OPFMM [CRG01]. OPLS [KB02, KOML08, KDSV02, MT03, POJ01, PB05, XLT07]. OPLS-AA [KOML08, POJ01, PB05, XLT07]. OPLS-AA/L [KOML08].
OPO [KZY09]. Oppenheimer [ZWZ09]. opposite [JSHG07]. opsin [RG02].
optical [Bou01, CZFH07, CTFC08, Hua09a, KSB09, LC09, LFR07, MA09, SN06, TKD07, WCL05, YFR05, Ze08, ZX08]. optics [MMP+07].

**Optimal** [GFS05, ÁCD+03, BSP06b, Blo04, CRG01, DDVD09, SPT07, TTBM09].
**optimal-parameter** [CRG01]. **Optimization** [Ano06c, GL04b, GKHO5, IK00, WCS09, WM12, AJ03, AM06a, BP00, BdPRMAI00, BM00, Bud07, BLMS08, CS02, CB07, COS01, CYM02, CLH+07, CY09, CY13, CHMI05, CMBC08, DMN03, DV02, FM00, FRLN09, GHMP03, HBBH00, HLTLP09, KKG+09, KBA+04, KHF+09, KK01a, LJKLM08, LJ04, LS05a, LS05, MKT04, MM03, MM00, MW00, MGJAA00, Pen06, PU09, Pul05, RK04, SCC04, SYC08, SWM04, SMMW09, SE08, SBH02, STC08, VMF+03, WS05a, WS02a, WPS02, XZZ04, YL06, YCS07, ZBS03, ZZ08, vLBBR12, WZW+06].

optimizations [IR03, PO03, RON02]. Optimized [KM07, VB03, VK06, BSDM04, FKF08, LIZ+07, MV06, MY08b, MY08a, WTKM06, WNH03].

optimizer [KG02]. optimizing [QSS01, SRC03]. **Orbit**
[Duk01, CR08, CR09a, DXW08, KRM+02, KTM02, LB08, LXSF08]. **Orbital**
[KIM+09, Pen06, WM12, ALTB06, AB09, AS00, CFK08, FOK+04, FK+06, FI+07, FKU+05, FMK+06, FMK+07, GCCB00, GS07, HHHW08, Hir08, IK08, IJK09, KDG+09, KBL08, KFK07, LKT04, Mas01a, Mas01b, MG00, MY08b, NYK+09, OS06, OO08, PU09, SRE08, SSMW09, TBGRJ04, UHHN09, VM00, WPH+07, vLBBR12, vdVDG00]. orbital-based [CFK08].
**orbital-correlation** [SRE08]. **Orbital-orthogonality** [Pen06].

**orbital-valence** [MG00]. orbitals
[ABF+03, Bac07, BME05, CVVB04, EdlVR+03, FMSA06, GFS05, GC02, HY07, ITN+05, Ish03, JHPRM+05, Kau07, Kni00, LW07, MS01]. order
[Bie04a, DSR+07, FS04, Gri03, IN08, JSHG07, KGN07, LAR+03, LS08c, May07, MO09, QTdG+08, Rud05a, Rud05b, Rud05c, YH09]. ordering [SM08a]. organic
[ATH+03, BLL+06, BT00, CCK01, DA01, EDA04, EBD+01, Go09, HELM09, HP04, JLLH03, JVKK09, JTR05, KLH+04, LH02, LJZ+07, LMRVFH+09, PO03, PB04, SJJ+04, SY+03, TAS07, Van02a, WCK00, YGZ05].
organizing [BA08, ZA07]. organocatalytic [WSM+09]. organocopper [YN03]. organometallic
FOK+04, FCK+08, UKN04, VSK+04, vGGB00]. parallelized
[TP01a, VK06]. parallelizing [SO07]. parameter
[BLMS08, CRG01, CHMI05, HXLS09, MO09, OVMV04, SHK+05, FM00].

Parameterization
[KB02, PNG08, SM+08, TCT03, BGJ01b, FH01, JKL08, JGH00, LSWB00,
MTE04, PB04, RKH03, TGLL07, VSW+03, WK01, JJB02, JVVK09].

parameterized [GB04]. parameters
[ABC00, AMR04, ANO06c, ATBLS04, BBG+04, BSDM04, BZL05, CYS02,
DB06, DDVD09, FAR02, FSFK05, FR505, HPL03, KFN08, KOML08,
KVL+04, KC01b, MMMYM, MSR04, MRC03, MLL08b, MC06, OYH05,
OMH08, OBT09, PRK05, RRCA08, SO09, SEKS09, SRS03, SSHD+08,
SCF+09, TT05, TTB01a, VCM01, VIP+06, WZW+06, ZSK07].

Parameterization [PDS01, COL01, SBH02, WS05b]. parametrized
[RSP03, TAS07]. paraoxon [ZWS+09]. parent
[MDI04, YLW+08]. Pareto
[STCJ08]. Paris [HP04]. Parr [Kri09a]. Parrinello
[JP09, Sch04]. particles [BS06]. partitioning
[ACD+03, DVP+02, DVR+03, HSM06, RP07a, VC04, WNH03]. path
[ABB01a, ABB01b, BLO04, BOS01, CY09, DF08, GWM08, JP09, KLI01,
Qua01, UCT+03, VGB08, WLPF05, WHG+07, CY13]. paths [FG03].

pathway [LGB+09, WLL01]. pathways
[AJ03, JW06, LZKT04, MAF+07, Qua04, RAGL09a, RAGL09b]. Pattern
[DHGR02, EKB02a, EKB02b, EKB04, AGMPRG+08, HWDB03, dGW01,
EKB02a]. patterns [CGG06, Gor01]. Pauli [Ish03]. PB [GC04, WHF08].
PBCAID [QSS01]. PBSA [PB06]. PtBIO [ZXYF09]. PC
[ANO01b, BMRRB01, HSM04, OS03]. PC-GA-ANN [HSM04]. PCM
[FKL+06, CR03]. PCs [HS07b]. P [DGD+05, GBBH09]. PDDG
[RCJ02b, TBGR04]. PDDG/MNDO [RCJ02b, TBGR04]. PDDG/PM3
[RCJ02b, TBGR04]. PDE7 [DD08]. pea [PS03]. penicillin [MK02].

penicillin-binding [MK02]. penicillins [DSS03].
pentacarbonylmanganese [PSS05]. penates [BPC01]. PEPCAT
[OML+00]. Peptide [Adv04, DHW+07, HJCP01, JPF+00, ONH00,
PFJ+03, BTP09, BWE05, BSP06a, CLWL09, CSJ01, CJSW+09, CLA+00,
CP09, DGV00, DWNB01, GB09, IGNH03, LHL+06, LL01, MS03, MHT01,
MST+08, OGH05, OKH+02, PHFC04, SLD07, TAT04, WCF04, WIL01b,
YZ06, YCBM00, ZALMG03, ZCZ03, WHP02, KVS+06]. peptide/HLA [KVS+06].

peptide/HLA-DQ8 [KVS+06]. Peptides
[CPML08b, Van08, ANO06c, BBHD04, BCP04, BAH+02, CP08, DJ04, EA08,
HHP04, IKYM09, LKJ+04, LLW02, LXL07, MM00, MC06, OML+00,
OYK+09, OO08, OM04, PCO+07b, PRK05, PFC03, SJW09, WZW+06,

peptide/HLA-DQ8 [KVS+06]. Peptides
[CPML08b, Van08, ANO06c, BBHD04, BCP04, BAH+02, CP08, DJ04, EA08,
HHP04, IKYM09, LKJ+04, LLW02, LXL07, MM00, MO04, OML+00,
OYK+09, OO08, OM04, PCO+07b, PRK05, PFC03, SJW09, WZW+06,
peptidomimetics [BAH+02]. peroxidative [MRS09]. peroxides [LLZL09]. peroxynitrite [JM07a]. personal [May07]. perspective [KRLD09, LMGO+09, PBF09]. perspectives [Fie02]. perturbation [CWY09, CPML08a, CG05, DRMD03, DSR07, FII07, Gri03, IN08, LKW04, MRS+07, NUH02, Ocs09, PMGL03, Pog06, QTdG08, RSE07, SWZS04, UTH+03, UKNS01, UKNO4, Var09, WCFH02, WHN03, YH09]. perturbations [OV03]. perturbed [DOSG06, ZZW09]. pesticides [KEH+02]. PH [RD00, DR09, WDS06, MCM04]. pharmaceutical [KV00]. pharmacophore [RA08, JFG04, LFKL00]. pharmacophore-constrained [LFKL00]. phase [BAL+01, CPJ00, CPJ01, DR09, DGI+08, DWC+03, FBDG06, FM00, GLMV09, JJK+00, JHZ09, KSB+02, KT08, KFNH08, KKH+07, LRI+02, Lee09, LB05, LL03, MFB04, Mas01a, Mas01b, MM02, Mor02, POJ01, PV07, wQZsLyZ02, QNF09, RRS06, ROC00, SMGE08, SDvG01, SMK00, TK08, TDH06, UCT+03, UNM+01, WD04, XKKL03, XKG+05, YQQH09, ZALMG03, ZSK07]. phase-space [QNF09]. phases [ALC08, CLP09, LXS08, SK05, XBJ08]. PhAST [HHG+09]. Phe [VKP+08]. Phe-Gly-Phe [VKP+08]. Phen [ZWS+02]. phenol [LL01]. phenols [HM08]. phenomena [KK08c, RSS09]. phenoxy carboxylic [KKKL03]. phenyl [WZY04]. phenylalaninamide [HJCP01]. phenylalanine [SMV+09]. phenylene [ASDP+06]. Philippe [Bi09]. phillipsites [LST08]. phonon [EL09]. phosphatase [AG00, FCP+04a, FCP+05]. phosphate [LDY+08, MBF+00, PPM05, PHRR08]. phosphates [WOC+03]. phosphatidylcholine [CEP07]. phosphine [HT05, LL00, MGLDS00]. phosphinine [LTF+07]. phosphinine-containing [FLOD07]. phosphinine-containing [FLOD07]. phosphininium [LTF+07]. phospho [RGP+07]. phosphodiesterase [XLZ08]. phosphodiesterase-5 [XLZ08]. phosphohistidine [KVL+04]. phosphomidazole [KVL+04]. phosphopholine [LFR07]. phosphopholine-containing [LFR07]. phosphophospholipid [MCR08, RG08]. phosphomannose [RGP+07]. phosphonic [CJK+02]. phosphorus [LYK+04, LTF+07, Mit01]. phosphoryl [ZJM+07]. phosphorylation [HLT+05]. phosphotriesterase
photoabsorption [CHRL09]. photoadsorption [ZMH09]. photocatalysts [HZ09]. photochemical [Ama02b]. Photochemistry [GD06, SRE08]. photodetachment [LMCD09]. photodissociation [JHPRSM05, LXSF08, WXX03]. photoelectron [VDM06]. photoemission [RDM08]. photoexcited [SRE08]. photographic [Sha02]. Photoionization [MY08b, MY08a]. photoisomerization [GRO03]. photosynthesis [Ano06b, CPM03]. photosynthetic [IN01, OON01]. photovoltaic [LMRVFH09]. phthalocyanine [CM09]. phthalocyanines [LS02]. phycobilisomes [MAF07]. phycocyanin [MAF07]. phylogeny [LXZ06, ZLY07]. physical [BRS07, DHW07, OFB08, OS08, SRCD03]. physically [AE06]. physico [AGMPRG08, Mat03]. physico-chemical [AGMPRG08, Mat03]. physico-chemically [SB01]. physicochemical [CP08, CP09, FTLV01, KLL04, KEM08]. physics [DBI02, SPL02, WS07]. physics-based [DBI02, SPL02, WS07]. physio [CDD02]. physio-chemical [CDD02]. piano [FKS09]. piano-stool [FKS09]. picture [VBGL00]. Piero [Ano06b]. pinacol [YT07]. Piotr [Ano06c]. pivot [ZYW09]. pK [KKS04, ZCS04]. pKa [CFR06, OS06]. planar [CSB08, MMRVH07, SRS07, SG09, Wav09]. Planck [DAK08]. plane [PSS04, PSMB05, RLD09, VSK04, XL07]. plane-wave [PSS04, VSK04]. plane-wave-based [RLD09]. planewave [YK08]. plaster [HP04]. Plastocyanin [SN06]. platform [Ga09, Gnu09]. plausible [CBS03, SB01]. play [YJF06]. Playstation [LEV09]. pleated [PG05]. Plesset [CPML08a, DSR07, FII07, Gri03, IN08, JSHG07, Var09, WCFH02, YH09]. plot [KMH02]. plots [CLZ09, SDL09, SRE08]. PLP [PMM05]. plus [AGMPRG08, CG05, IKN08]. PM3 [BM00, BSDM04, DC02, GM01, MSH06b, RCJ02b, TGLL07, TCT03, TBGRJ04]. PM3-compatible [BSDM04]. PM3/d [TGLL07]. PM5 [LK04b]. PMF [Mue01]. pocket [BS08, MD08, OH09]. pocket-specific [BS08]. Point [Est07, BCNs07, Bie04a, CRC08, DVC03, GGR00, KLG07, KKL08, KF03, MGCA07, SRB02, TBS09, WMS06, ZMH09]. point-charge [DVC03, GGLR00, SRB02]. points [BMLV04, BAA07, DLD02, GMA04, HQ02, MP03b]. Poisson [WB04a, WB05, ABW09, BWH00, BH03, BF04, BF07, DLS00, DAK08, FOL04, GP01, GCD08, GGT08, H0505, HB00, HB01, KWH07, LDG02, NYT09, PS04, SAT04, Vas02, VZM08, WBO4b, ZGFL01]. Polanyi [Nye07]. polar [BAA07, CYM02, CPML08a, EB04, FA01a, HLL06, HS08, JPF00, PFC03, ZXY09]. polar-neutral [CYM02]. polarisabilities [ZPL07]. polarisabilities [ZPL07]. polarizability [FROD08, LFK05, LYS08, MLA00, MY08a, SKK07, Tor02, WHE08]. polarizability [BP01, HK08a, HK08b, Mar03, Mor02, QCK01, QCK02, VGBK00]. Polarizable [CFK08, LL09, Nak07, Ano06c, AG08, AP05, BCIB05,
COL+06, DGI+08, FKL+06, GWM+00, GS04, GKTS04, GPK05, HHP04, JZD+09, KSB+02, Kol04, LJ04, MMPK01, MBC08, OR05, PWHF+03, PWHF+04, Pom04, RGP+07, TFZRG01, WZW+06, YGLvG06, FCP+04b].

**polarization** [CGB03, CBH+03, EDW07, GGLR00, GKTS04, HK08a, HK08b, KFZ03, MR04, Maz08, RP02, SL09, WL09a, YL09].

**Polarized** [EdlVR+03, BSOB05, OBBS05].

**poly** [ASDP+06, BSJ01, CHA+07, CFD04, MGMM07b, Qua07, SBB02, ZALMG03].

**poly-isothianaphthene** [CFD04].

**poly-para-phenylene** [ASDP+06].

**polyacenes** [BPCD07].

**polyacetylene** [PM02].

**polyacrylates** [LZA02].

**polyalcohols** [KBLP09].

**polyatomic** [GGB07a, GGB07b, RLER04a].

**polyatomics** [TP01b].

**polyazidocubanes** [JWB05].

**polycoordinated** [TGGP+00].

**polycyclic** [Bor03, CA07b, FVB08, MGMM07a, VS08].

**polyenes** [MW09].

**Polyethylene** [BCF+09].

**Polyketides** [KB02].

**Polymer** [Mei02, BBG+04, CZA03, DJT08, MM07, RRZA08, YSJ09].

**polymeric** [Fau01, JCA+02].

**polymerization** [BG07, YXC+07].

**polymers** [CFD04, CA04, CA07a, DC02, Der09, Din00, DDBP09, HM01, LAEL01, OKE+02, SHH07, VIP+06, YYW07].

**polymorphism** [VVBV02].

**polynomial** [HDBD04].

**polynuclear** [HYR06, RRFC+03].

**polyoxoanions** [LFR+04].

**polypeptide** [Cri04].

**polypeptides** [CPML08a, IB04, KF02a, KF03, Nak02, VP09].

**polyphosphate** [MRC03].

**polythiophene** [CA07b].

**POPC** [JM07b].

**Pople** [Ano04a, EA08].

**population** [BLT03, BPCD07, Pul05].

**population-based** [Pul05].

**populations** [KB02].

**porphin** [SBL05, SBL05].

**porphycene** [NyHN06].

**porphyrazines** [LS02].

**porphyrin** [AZM03, CHRL09, LPP06, NyHN06, NHN06].

**porphyrin-fullerene** [CHRL09].

**porphyrins** [CN05, LS02, LWH06].

**portable** [SH07].

**pos训rit** [RGG08].

**Possibilities** [PRDS08].

**possible** [LMGR05, LBG08, TT05].

**Possible** [HIA03, OCP02, WLL01].

**post** [WW03].

**post-HF** [WW03].

**posteriori** [SPDS01].

**potassium** [MCR08, MHS05].

**potential** [AMR04, AE06, ABCC01a, ABCC01b, BCNs07, BL05, Bof01, BBI+09, DMLI05, DMC05, DLHC06, DK01, FSFK05, FKRE08, HPP00, HRBKB03, HPL03, HFSD03, IS03, IT03, JZD+09, LFK05, LMK01, LS08c, MMLC05, MCF05, Nak07, NG04, NAMM01, PSC+01, Qua01, RD06, RNG03, RHL09, RTG00, SPDS01, SS00, Sch03, SMGE08, SSS+09, SHH07, SG07b, SBB02, SJW09, TBSM09, TLKT00, WCC08, WL09a, WCK00, WS07, YH06, YHD+06, ZCS04, ZZY07, ZZY08, ZGXX06].

**potential-derived** [TBM09].

**potentials** [ATM+07, CLC09, CPUGD09, CKW09, DBI02, FAB+00, FNP+06, GK09, GBJ03, HZ04, HHH01, HZ06a, IKYM09, KLH+04, KCK+08, KK01b, LJ07, LHI09, LK03, LKO4, LLW+09, MCF05, MWE02, OR05, PML03, RPMP03, RLER04b, SMM00, SPT07, VGDS08, dSR08].

**Powder** [HWD03, HH03, dGWH01].

**powerful** [PSDM00].

**pp** [Bic09, Lip00, Sta00].

**PQS** [BWM+09].

**Practical** [BMRRDB01, PRR+05, W001, You11, BLO04, Sch03, SHS05, SWZ04, WW03].

**precalculated** [ZMZ09].

**preceeding** [CSD05].

**Precise**
[Ami00, Ara04]. **precision** [CN03, GAAdGM08]. **precursors** [CFD03, CFD04, DJT08]. **predict** [HL08, HZo06a, HZo06b, LL07, PB06, PJPdPRMI07, XSHC06, XLCO8, YMT04]. **Predicted** [PDP02, IGL07, JARM02, KCL06, WS02b, ZCL09, ZGXX06]. **Predicting** [AVS09, CLC03, CKR08, CJDK09, DA01, ELK+09, FCW06, G09, JIK09, KLM+04, KCK+08, KEH+02, KF03, KKS04, LCC09, NINAT+07, OFB08, Sch00, YCW+09, YYW+07, AB04, BED02, CLF+09, CLA+00, DO6, EK06, GP06, GAS04, HEP+02, HMSM06, HG08, KZ09, KP05, KFNH08, KEB04, KK08b, K08, KOFF09, KF02a, LEK07, LXW+09, LHP01, LLZO9, LWW+09, MSF+08, MS04, NCO+05, NLL+09, PJ+07, QHL09, RGG08, TKS+01, TLKT00, Tot04, VGDSU08, WFHP01, WHP02, WHF08, WX09, ZHH09, AGI+07, GCD+08, KS+06, ZCS04]. **predictions** [BS01, BLB09, CP08, Ruv07, VVan02a, ZLD09, vEMK01, vE01]. **predictor** [Kol04]. **preface** [FA01b]. **preferences** [GSB09, KK09, LKJ+04]. **preferred** [DV02]. **preliminary** [KMH02, PMC+08]. **Preprocessing** [SHM04]. **prerequisite** [WHF08]. **presence** [LZA04, RAGLL09a]. **present** [GR07]. **Presentation** [Rud05a]. **preserving** [QNF09]. **pressure** [Car02, MTB09]. **pressures** [TK08]. **primary** [KB09, JIK09, KBN02]. **primitive** [MV06]. **principle** [GJL+08, PRS04, ZDS+05]. **principles** [CS01, EBL+08, GD09, HZX04, Hua09b, K08c, MLJ03, TK08, VP08, WLX+05, WZZ+09, WD08, ZXYF09, ZHMW09]. **prion** [IIK09]. **priori** [SPDS01]. **prismatic** [WL09b]. **probabilistic** [PJ+07]. **probabilities** [DP04]. **probability** [CFS03, DLW06, GCDL+05, Kn00, SK09, SCS07]. **probe** [CVR08, DMLI05, TH02, VSW+03]. **Probing** [PAT+09, WMGK07]. **problem** [ABB09a, ABC09b, Bof01, CCL06, HLTLP09, Qua01, ST06, TKH07, XOW+00]. **problem-size** [HHTLP09]. **Problems** [You11, ABWT09, Mat03, Vis02, Woo01]. **Procacci** [An06b]. **procedure** [AJ03, BBM+09, BAH+02, DRMD03, GRCD01, Gly06, GM04, IS07, Kli01, KWK+00, MP03b, ME06, PPXP01, PRJ02, QSS01, RMH03, SFRS01, SMZW05, TRS02, UHN09, UB07, VCK09, Zer08, BBC+05, BKS02]. **programmable** [G09]. **programming** [SP+07]. **programs** [CCD+05, KS08, MBP09, SH07]. **projection** [FS00b, GKH05, GY06, Qua04, TK+08]. **projector** [MOP+07]. **projector-augmented** [MOP+07]. **prokaryotes** [WHH+06]. **prolapse**
promising [SRJ01], promolecular [Leh06], promolecule [MS00], promoted [SBG09b], promotion [KMM07], propagator [SVT09], propenal [RR05], propanone [RR05], propargyl [LMK01], propellanes [PAS07], propenal [FDSA00], propene [BS03], properties [AB00, AEE03, ACD03, Ara04, AZS04, BG03, BZP09, BT00, BSOB05, BACJCT01, CMJ08, CDGS09, CDS09, CPDHZ08, CLC09, CVRI08, CZFH07, CDD02, CHA07, CRSB03, CTFC08, CMA08, DD08, DXW08, DWNB01, DVP03, D000, DPM09, DSS03, DHW07, EM03a, EM03b, Fan01, FTLV01, GKR08, Hua09a, HJCP01, JPF00, JXJ08, KHY00, KLT04, KJP07, KCL00, Kri09a, Kri09b, KG06, KPKZ06, KKL01b, LTF07, LWLS07, LC06, LFR07, LLZL09, LMRVFH09, MV06, MM02, MA09, NA06, NNAT07, NAT07, OBBS05, OS08, PMB04, PK04, PBF07, PTC01, PSS04, POJ01, RKA09, SRK00, TZX01b, TZX01a, Tor02, TDK07, UM03, VB09, VKCK09, VP08, WLX05, WM06, WCL05, YFR05, ZY01, ZXYF09, ZWP08, ZH08, ZSK07, ZMH09].

properties-based [VB09], property [BAA07, JLHF03, NLL09, PSCD09].

propylene [QZL04, RR05], propynyl [Lee09].

protease [BWE05, CLXC02, DLG00, LZ05b, NLL09, SPT03, SVV08, WHF08].

protease-inhibitor [SVV08]. Protein [LEK07, NCO05, PJB07, ADM06, AG00, AHG09, BED02, BRDC02, BMLV04, BS01, BSO6b, BS05, BSH07, BLMS08, CCC03, CLCX02, CLC03, CLWL09, CLS09, CIB05, CLH07, CR08, CLF09, CJDK09, yckHun08, CRH07, CPUGD09, CSRST04, DHM03, DPR05, DB06, DBI02, EBAN07, FOL04, FC06, FKM06, FKM07, GLD08, GHH07, GL04b, GC04, GDPCPU07, GdSuM07, GHMP03, GKK07, GZM09, GB04, HEP02, HFS07, HP01, HSO1, HML06, HLTL09, HLM05, HLT05, HZ06a, HZ06b, HGO8, HW09, HP05, ILTK09, IM06, IOK09, IT03, J07a, JMD02, JIK09, KFB05, KFNH08, KLS02, KCL06, KHF09, KK01a, KIFK07, KH05, KFO8, LFBSK07, LH07, LJJL08, LV08, LKZ04, LXW09, LL07, LW06, MFB04, MTK04, MLG04, MH09, MS02, MWE02, MLL08a, MHT01, MPF00, NMATA01, OFBO08, OFIK09, PB06, PRR05, PC00, PFC03].

protein [PSHP08, PMM05, PB02, PF06, PNG08, QLHL09, R08, RSER09, RLP08, RS08, RK05, Ruv07, SHM04, SLC09, SWM04, SWV05, SN06, SR09, SMG09, STC08, SL06, TLKT00, TDG05, V004, VW04, VGO07, VGDSU08, VGMM05, VSM08, WS05a, WS07, XZZ04, XSHC06, XLC08, XWC09, Yan04, YLO6, YFMS07, YPNE09, Yos02, ZP03, ZGFL01, ZS04, ZZ08, ZTS09, ZM06, dSR08, HLC09, PMB04, ZZTS09]. protein-DNA [PSHP08].

protein-environment [HFS07], protein-acceptor [LXW09, RK05].

protein-tyrosine [AG00]. Protein/solvent [PMB04]. proteinogenic [IKYM09].

Proteins [LMH09, AG03, AN06c, BBHD04, BCP03, BHH09, CR02, DWNB01, DNM03, DR07, DV02, DJ04, DJB02, DW03, ES00, ENM04, FNP06, GAS04, HB09, HHHS01, HM02, HS01, HHW03, HL08,
HJCP01, Ike04, IDMC09, IN01, KSB+02, KT02, KKS04, LR03a, LHJ+06, LKA01, MK02, MSH+06a, MZL08, NAT07, OS06, OSHS03, OM04, PB04, PMB04, PRJ02, RZGM09, RON02, SL09, SPL+02, SHBD05, SHSF05, SMV+09, VBS09, WZW+06, WM06, WS05b, WHH+06, XZ05]. Protocol [AGI+00]. Proton [SRB06, AGK03, BA03, BA04a, CXZ+09, FDSA00, FO08, GWM08, HFHL06, LLM08, LMGO+09, LB05, MA05, PGG06, PCS04, SM06, WFHP01, WHP02, XKG+05, ZCS04, dSGCG00]. proton-coupled [CXZ+09]. protonated [CPDZH08, ZDS+05]. protonation [Bac05, CG05, DHM+03, HP05, KYFW07, WHF08, XZ05]. protoporphyrinogen [WZY04]. prototype [Ang09, CS01, ASDP+06]. prototypes [SSS+09]. proximity [Agr03]. pruning [TCSM03]. pseudo [LL07, VDM06, XSHC06, XLC08]. pseudoknots [DP03, DP04]. Pseudomonas [NYK+09]. Pseudopericyclic [LFS+07]. pseudopotential [FMAMVK06, LK03, VW03, vW06]. pseudopotentials [PSS+04, PSMB05, SMD02]. PSI3 [CSV+07]. psoralen [NBTN04a, NBTN04b]. Pt [DMN05, LWK08, LF02, RD00]. PtCl [LF02]. PtF [LF02]. Pu [Han01]. Publisher [Ano04a, Ano04b]. pump [CVR08]. pump-probe [CVR08]. PUPIL [TdMSD+08]. Pure [WG02, Rud05a, SDCG02, SCP08]. purpose [DGI+08, JGVF05, KAK+09]. Putting [MDI04]. pVDZ [Wib08]. pVTZ//MP2/6 [WD04]. PW [EBL+08]. PyFrag [VGB08]. pyrazine [LWX07]. pyrazole [DMC05]. pyrazoline [LLKC06]. pyrazolyl [HT05]. pyrene [HIA03]. pyridine [CHA+07, HT05]. pyridines [WRP+06]. pyridoxal [LDY+08, PMM05]. pyrimidine [LWX07, XWXC08]. pyrimidinyl [WJX+08]. pyrolysis [KKH+07, XKKL03]. pyropane [ZWTP+08]. Pyruvate [CJPZS08]. pyVib [Zer08].

Q [BS08, KWK+00, WHG+07]. Q-Chem [WHG+07, KWK+00]. Q-Dock [BS08]. QCISD [ZKZ+07]. QCT [DPM09]. QM [CGBF05, MPF00, AGK03, AST06, AB09, CR09b, CG05, FAR02, FMSA06, FSFK05, GWM08, GWM+00, HHHB00, HBM06, HNR08, HRR05, HT03, HTN03, IV04, IvSV06, ITS05, ITS06, KHF+09, KBLP09, KPR04, Kr08, Kr09b, LLL03, MMB+00, MK02, MSH+06a, MG00, MLJ03, NGTB03, RG02, SURG06, SSB+99a, SN06, SMM+08, SVV+08, THHN01, TdMSD+08, VMF+03, WCC08, WHG+07, WC08, ZWZ09]. QM/FE [AGK03]. QM/MM [CGBF05, MPF00, AST06, CR09b, CG05, FAR02, FMSA06, FSFK05, GWM08, GWM+00, HHHB00, HBM06, HNR08, HRR05, HTN03, IV04, IvSV06, ITS05, ITS06, KHF+09, KPR04, Kr08, Kr09b, MBB+00, MSH+06a, MG00, MLJ03, NGTB03, RG02, SBB+99a, SN06, SMM+08, SVV+08, THHN01, TdMSD+08, VMF+03, WCC08, WHG+07, WC08, ZWZ09]. QM/QM [AB09, HT03, SURG06]. QMCF [PHRR08]. Qmd [KMH02]. Qmd-plot [KMH02]. QMPFF3 [DGI+08]. QMQSAR [DML05]. QSAR [DHW+08, DHW+09, SGPS09, CGMPT+08, CMBC08, CRGN07, DML05,
DMC05, GDPP08, HSMT04, HMMS09, LLL+08, LJZ+07, LSY02, MRS09, PS09a, SJ+04, TCSM03, VB07, VB09, VGDSU08, XYN+06, ZNLL07.

QSAR-analysis [VB07]. QSAR/QSPR [TCSM03].

[CDGS09, CDS09, CDGS09, GS08, HM08, TTBM09, TCSM03, ZNLL07].

QSPR/Q SAR [ZNLL07]. QTAIM [MGMM07b, RKA+09]. quadratic [ABBQ01a, ABBC01b, Bof01, HG08, Qua01, ZHH09]. quadrature [CG06, DBS08, GC03]. quadrilaterals [GKK07]. quadrupolar [CMA08]. quadrupole [HLLN06, HK08a, HK08b]. quality [BG03, CMJ08, EM03b, FKZ09, JBJB00, JJB02, SSS09, TSSGS07]. quantifying [GT03]. Quantitative [Mit01, WZY04, YNZ+08, BAA07, CDGS09, CDS09, DHW+08, DHW+09, Gra07]. quantization [GLMV09]. quantum [WOC03, XYN+06, XZZ04, XLZ08, ZC03, ZAT07, ZSK07, SB08, CGB05, DSS03, KBL08, FBN05, SCS07]. quantum-chemical [DA01, SFRS01, VCK09, XYN+06]. Quantum-connectivity [EDAJ04]. Quantum-regions [SB08]. quartet [MSBS01]. quartet/metal [MSBS01]. quartets [MSBS01]. quartic [SAS05]. quartz [ZW04]. Quasi [AGI+07, NUH02, AGI+00, ITN+05, VMA03, YH07]. quasi-canonical [ITN+05]. quasi-degenerate [NUH02]. quasi-flexible [AGI+00]. quasi-relativistic [VMA03, YH07]. Quasirelativistic [HWFN01]. quaternary [CW02, SO07]. quaternions [CSD04, CSD05, Kne05]. Quick [LMV07]. QUICK [SB08]. quinolines [KS05e]. quinoprotein [JHH01]. quintet [GW01].

R [Bof01, CPJ00, LZZC09, Lip00, Qua01, ZY01, LZZC09, ZPL07]. rack [OC02]. Radical [GC03, ESP04, Kau07]. Radical [XDS06a, AV00, BL06, CUS00, CUS03, CXZ+09, GBS09, HIA03, JDWS06, KOM08, KKMS04, LC07, LMK01, NSB08, O004, gThDjL01, WDWS06, WDS06, WDS07, WyLG+09, WLZ+07, WLL+03, XDS06b, YLWL09, ZLSS04a, ZLSS05, ZLSS06a, ZZ+09, CXX+09, QZZZ03]. radical-molecule [ZLSS06a].

radicals [BE07, Dib05, Lee09, WLLS04, WDS07, WSC09, YLW+08, YLWL09, ZM03]. radii [OB02, PML03]. radon [HD06]. Raf [GC04]. Ramachandran
[SDL+09, GSB09, HHP04, PFJ+03]. **Ramachandran-type** [SDL+09].

**Raman** [Bou01, LC09, NRKH02, OBBS05, Zer08]. **RAMSES** [BMRDB01].

**random** [CY09, CY13, CA04, HXLS09, JS07a]. **randomized** [LFKL00].

**range** [CEP07, GPK05, Gri06, HGMB04, IZA06, JPCA08, KSS08, MN02, RP07c, RLP08, San01]. **range-separated** [JPCA08]. **rank** [RP07c].

**Rapid** [GGA00, RSN+02, BH03, Gra07, KMH02, KC01b, WS05a, PABK03].

**Rapidly** [KF02b, Zho06]. **random** [CY09, CY13, CA04, HXLS09, JS07a].

**randomized** [LFKL00]. **range** [CEP07, GPK05, Gri06, HGMB04, IZA06, JPCA08, KSS08, MN02, RP07c, RLP08, San01].

**Ramat** [GGA00, RSN+02, BH03, Gra07, KMH02, KC01b, WS05a, PABK03].

**Ramachandran-type** [SDL+09].

**Raman** [Bou01, LC09, NRKH02, OBBS05, Zer08]. **RAMSES** [BMRDB01].

**random** [CY09, CY13, CA04, HXLS09, JS07a]. **randomized** [LFKL00].

**range** [CEP07, GPK05, Gri06, HGMB04, IZA06, JPCA08, KSS08, MN02, RP07c, RLP08, San01]. **range-separated** [JPCA08]. **rank** [RP07c].

**Rapid** [GGA00, RSN+02, BH03, Gra07, KMH02, KC01b, WS05a, PABK03].

**Rapidly** [KF02b, Zho06]. **random** [CY09, CY13, CA04, HXLS09, JS07a].

**randomized** [LFKL00]. **range** [CEP07, GPK05, Gri06, HGMB04, IZA06, JPCA08, KSS08, MN02, RP07c, RLP08, San01].

**Ramat** [GGA00, RSN+02, BH03, Gra07, KMH02, KC01b, WS05a, PABK03].
[Adc04, GKK07, KLS02, RS08, TGD05, WG02]. recoverin [LGB+09]. red
[McD08, SRK+00]. red- [McD08]. redesign [GLD08]. redistribution
[ZY01]. RedMD [GSDT09]. redox [GK09]. Reduced
[BR04, BSOB05, OBBS05, ABBC01a, ABBC01b, BMLV04, Bofo1, CNN07,
CP08, DLD+02, EI07, GSDT09, HP01, Qua01, RS08, WEE01].
Reduced-size [BSOB05, OBBS05]. Reducing [PRSMM02, SSL02, SY09].
reductase [CFER04, GGB+09, CBC+08, DBS07, GGLR00, HLLN06, LPP06,
PCS04, PFR04a, PFR04b, TMBM02].
reduction [CCCJ09, DBS07, DMN05, HLTLP09, LRWG03, Mck07b].
reductive [PS03].
reevaluation [Kle03]. Reference
[ZZ08, CF04, CFC+08, LZ05a, NUH02, OV03]. Refinement
[HB09, Ruv07, BHW00, MM05]. refinements [GPK05]. Refining
[CLWL09, SB01]. refractive [YYW07]. regarding [KZ09]. region
[ABWT09, Ama02a, HHHB00, WEE01]. Regional [TKH03, NTH09].
regions [HYT05, SB08]. regioselectivity [AVB00]. Registering [GBL+05].
regression [DLWV07, Gol09, GS08, LCC09, SY09]. Rehybridization
[AM07]. related [ALC08, ACLD03, CFD04, KC01a, LXW+09, LWH06,
LCDA03, LCGA03, LCA03, ML00]. Relation [SM08a, DVRP+03].
relationship
[DHW+08, DHW+09, JPCA08, KWK+01, WLI+05, KWK+02].
relationships
[BAÁ07, CDGS09, CDS09, CPUGD09, JLHF03, PSCD+09, WZY04].
Relative [SWV+05, BLB09, CG05, MML+06, MRS+07, RSE07, ZOJ+06].
Relativistic [FHF+01, NYH02, NSO+07, SNM+06, SMD02, WTKM06,
YH09, ASS+02, BBI+09, Dya02, GHLK+02, GSP06, HDMdS05, Hs06,
HD06, LF02, SH02, Van02b, VMA03, WL02, YH07]. relax [GFS05].
relaxation [BRDC02, HS01]. relaxed [AEE+03, CA07a]. relevance
[Ano06a, MGCA07, ST06]. reliability [IB04, LKW04].
reliable [BE06, WHF08]. remove [LZ05a]. removing [PCS04].
reordering [TVL+03]. reorganization [FZL+06, KMM07]. repair [Pin03].
reparameterization [RFSS06]. repeat [NK01, NL08]. Repeated [KH01].
Repeated-annealing [KH01]. replica [FSM09, FGR07, GLP08, NCO+05].
replica-exchange [FGR07, NCO+05]. Reply
[Bofo1, CPML08b, WM12, CSD05]. Representation [GPK05, BB08,
CRK08, CF06, JIK09, LW04b, LXZ06, LW06, RLR+04, WE01, HYDN+08].
representations [BMLV04, LAR+03, LR06, RS08, SN00, YNW05].
representative [YLL+09, YXL+09]. reproduce [VBS09, WS05b].
reproducing [MF04]. repulsion [COL+06, Kri09a]. repulsions
[HGM04, PB09]. repulsive [BDW00, CFC+08]. requirements [AM06b].
research [JLHF03, PGH+04]. residual [RI08]. residue
[MH09, NBTN04b, PMA06, NBTN04a]. residues
[CFS+09, DHW+07, HJCP01, JPF+00, OS06, UNHYT06, XLT07].
resolution [BSO5, BS08, CDGS09, DSR+07, GL04a, HXLS09, Nee03,
WMRW+01, WS02b]. resolution-of-the-identity [DSR+07].
resonance
resonances [LMB08, PF06]. **RESP** [WCK00]. respect [QCK01, QCK02] response [HG08, OFIK09, vGGB00]. Restrained [SRB02, WCK00]. restraint [LI07, LHI09]. restraints [BS08, HWTL03], restricted [BdPRMAI00]. restrictions [KSB09]. results [CSD05, LKT04, PFJ+03]. **Retardation** [HP04]. retention [RC04]. **reticulum** [HLB09]. retinal [BL05, LFEdL06, MSH+06a]. **Retrieval** [CVR08]. reuptake [FFG+06]. reveal [DLRZ09]. revealed [HW09]. reveals [Pin01]. reverse [AJNG01, ML00]. Reversible [DvG00, Kol04, NHN06]. Review [Bic09, CvG08, Sta00, Sta00, Woo01]. Reviews [LB99, Sta00]. Revised [ATM+07, SBB02]. revisited [ASY01, CVVB04, PCS04]. Revisiting [GPSP06, JPCA08, LN01]. **Rg** [ZXY03, ZXY03]. RGF [HQ02]. Rhenium [SBH02]. rhodium-catalyzed [GLH+08]. Rhodopseudomonas [IN01, OON01]. rhodopsin [CEP07, YKK09]. Rhodopsin- [YKK09]. ribonuclease [KSK00, WOC+03]. Ribonucleotide [CFER04, HLLN06, FCS04, PFR04a, PFR04b, TMBM02]. ribose [SA07]. ribosomal [SB01]. ribozymes [MMMY07]. rich [CZ05, LWK08]. Rigid [SM03, DPRR05, Din00, ECA06, FS98, FS00a, Ike04, Lehl06, LV08, KP05]. Rigid-body [SM03, Ike04]. **Ring** [ZSE08, BE09, CDPL09, DC02, DLSVY00, FJ08, RNJ07, SRE08, ZW09]. ring-structured [DC02]. **RISM** [MH08b]. rival [DDVD09]. RM1 [FBL08, RFS06]. RMSD [Kne05, CSD04]. **Ru** [Wei08]. **RNA** [AM06b, DW08, GdAcV+07, LHWX07, LCSZ09, LOL+08, MB00, Mak08, RTG00, SB01, YNW05, ZZTS09]. RNA-ligand [AM06b]. **RNAcluster** [LOL+08]. **RNase** [RWBH09]. ro [LN01]. ro-vibrational [LN01]. robust [GS08, HEP+02, YK00]. **ROCR** [CPJ00]. rod [BCIB05]. rod-like [BCIB05]. **Role** [BCF+09, CPJ01, CFS+09, CPF02, Ru0v07, SVV+08, ZSC05, BY06, CDS09, CFER04, Kau07, TFZ001, VBGL+00, YT04, YTY07, YJF06, PMM06]. **Roles** [ALC08, IN01, NYK+09]. roll [FS98, FS00a]. **room** [TD08]. Roothaan [TW03]. roots [BdPRMAI00, Nil09]. **Rotamer** [HLTLP09, GHMP03, KBLP09, LFBSK07, SMG09]. **Rotamers** [LMH+09, SHM04]. **rotation** [CMLS05, COMR+04, DHF+05, DBM03, HFSD03, HK08c, LHI09, LZ05a, MGL03, OMNH08, PB09]. **Rotational** [CSD05, BVW04, KBN02, TSS05]. **rotations** [IR03]. rotors [WR07, WFR08]. rough [Pan07]. rough/fractal [Pan07]. roughness [PHJ+08]. routes [GGGL05]. routine [Kli01]. routines [AT02]. row [AD00, BP03, BG01b, JGH00, LK03, LK04, RRP+01, YTH01]. Royal [LWW+06]. **RS** [RAR+03, EKO06, ELK+09, KEH+02, LRG03]. **RS-HDMR** [LRG03]. **RT** [TYO+02]. **Ru** [ZWS+02]. rule [GR07]. rules [AMR04]. runs [EL07]. **ruthenium** [FKS+09, PHKG07]. Rydberg [PRSMV08, ZM03, dSVA+09].

S [BSB05, Bic09, Gog08, HKHN08, JJK+00, KYFW07, MGL03, Mck07a,
LW06, LOL⁺08, LLL07, MHT01, WPH⁺07, YNW05. Section
[Ano01c, Ano04b]. sections [MY08b, MY08a]. seedling [PS03]. segment
[YS00]. segmented [CGSST06]. segments
[BTLP03, GAS04, KFO2a, YMT04]. segregation [Sza08]. Selected
[BMC07, Mat03, PRSMM02, ZOJ⁺06, LSAS01]. Selecting [HXL09].
selection [HW09]. Selective [TCSM03, XPW09, AM06b, MHL⁺09].
selectivity [BSP06b, GLRL02, OO08, ZVRC08]. Self
[ZA07, BA08, BWI⁺02, ECM⁺03, NUH02, NTH09, NL08, SH07, TKH03,
VTT⁺08, WM04, XL02]. self-associative [NL08]. self-consistent
[BWI⁺02, NUH02, VTT⁺08, WM04, XL02]. self-contained [SH07].
self-interaction [NTH09, TKH03]. Self-organizing [ZA07, BA08]. semi
[BBH04, UKN04, ZNNL07]. semi- [UKN04]. semi-empirical [ZNNL07].
semi-implicit [BBH04]. Semiautomatic [PRJ02]. semibullvalenes*
[HWGB01]. semiclassical [KM07]. semicore [HZ09].
semidirect [MBWP03]. Semiempirical [Gri06, LKT04, TT01, BUMCMRL00,
BM00, Der09, DMLI05, FBL008, FO08, GGLR00, HMO07, IK00, JFG04,
KSS08, KBT03, LMMW04, MAF⁺07, MS06b, MHT01, Nye07, RSSKB03,
RCJ02a, RCJ02b, SBL05, TCR⁺02, TBGRJ04, vVGD00]. semiempirical-DFT
[Der09]. Semiglobal [DV02]. semimicroscopic [KK08b]. semirigid
[CLP⁺05]. sensitivity [HLSH05]. sensitization [Sha02]. sensitized
[KS05c]. sensors [BBG⁺04]. Separable [EA06]. separated
[JPCA08, MLL06, WSM⁺09]. separating [CN03]. separation [FBGD06].
sequence [AM06b, CCWH02, CKR08, CLZX09, Dya02, JIK09, LXZ06,
LSW⁺01, PRJ02, WHH⁺06, ZLY07]. sequence-dependent [LSW⁺01].
sequence-specific [PRJ02]. sequences [CP09, DLW06, DLWV07, Der00,
JK09, LW04b, LD06b, LW06, MCF07, PP08a, hYDN⁺08]. sequential
[TT05, ZGZX07]. SER [JP⁺00]. serially [KMA⁺07]. series
[CC07, KML02, PDS01]. serinamide [PFC03]. serine [OB09]. serotonin
[HLC09]. serve [Mck07a]. set
[ABF⁺03, ALKH04, AHK02, BR04, BT00, BS0B05, BRV⁺07, BRL08,
BRLS12, CM08, Cho01, DMZ08, EL09, EKB02a, FZL07, FMP08, GGT08,
HdMs05, HMSN06, IO08, JKK⁺00, LFK05, MV06, Mas04, MLL⁺08b, MC06,
PSE⁺01, PRK05, Pen06, PFJ⁺03, PSMB05, RRP⁺01, SS⁺03, SHK⁺05,
TW03, VKP⁺08, VRT09, VKCK09, WMG07, Wib04, WG02, WZPR⁺04].
set-up [GGT08]. sets
[BY06, BS0B05, CR0S05, CUL04, EA08, EdlVR⁺03, GKH05, HdS06, HD06,
IO08, KKO08a, LST08, LTV08, MV06, NSO⁺07, OBBS05, OVMV04, RLA01,
RLE01, RLR07, SNM⁺06, VB03, WTK06, Wei08]. setting [HP04].
setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].
SG [CG06]. SG- [CG06]. SGB [GZL02]. SGB/NP [GZL02]. SH
[Mas01b, MGLL03, Mui05, SSS⁺09, WLLS05]. SH/ [SSS⁺09]. SH3
[IGNH03]. Shaik [Bic09]. shake [KFD06, BL09, FS08, FS00a, KVG01].
shake-up [KFD06]. Sham [Bou00, RRS07, SH02]. Shannon [LM03]. shape
[BR07, PRDS08, WM06]. shape-based [PRDS08]. shaped [LWW⁺06].
Shapelets [PRDS08], shapes [BR07, KS02a], shaping [HJCP01], shared [Sim07], sharing [BRS07, RS07a, RS07b], SHARPEN [LMH+09], Shaw [Ano05b], sheet [KF03, PP08a], sheets [LLW02, PGC05], shell [DSB+02, FS02, FO08, HB09, PRSMM03], shielding [CDL06, CDPL09, HWFN01, MC06, PF03, WZY07, ZPL07, ZXY08, ZLD09], shift [Dra00, HP05, LFZS04, MA05, RG02, WPS02, XZ04, ZFL+05]. shifted [McD08], shifting [CPFL02, HRG07], shifts [CDL06, CDPL09, HWFN01, MC06, PFC03, WZY07, ZPL07, ZXY08, ZLD09].

SHOP [XNC+07], SHOP-type [TYN05, GP05, HGMB04, IKYM09]. Short-range [GP05, HGMB04]. Short-time [TYN05]. shorter [MST+08]. Si [BSB05, TK08, WZZ+09, YHD+06, CJS+03, SURG06, WL09b]. silica [Unhyt06]. SIBFA [PWHF+03, PWHF+04, ROG00], SIBFA-LF [PWHF+03, PWHF+04]. side [DLHC06, ENM+04, GT03, HFH06, JPF+00, KG02, LL01, MT03, MMLC05, PF03, SMG09, VM02, XLT07, ZM06]. side-chain [ENM+04, GT03, JPF+00, KG02, MT03, PF03]. sieve [PHH+08]. sieves [LMV07]. SiF [LAT05]. sigma [JFG04, KMM07]. sigmatropic [LLKC06, LFS+07]. SiH [ZZL+09]. silastannation [WCHW09]. SiLi [XFF06, HXD08]. silica [SDCG02]. siliceous [LLT08, LTV08]. silico [LLW+09, MHW04, PHR+05]. silicon [BSB05, HXD08, KZW+05, KS01b, LB08, NBJ04, ZLI03]. silsesquioxanes [JW00]. silyl [MGG06]. silylenoid [XFF06]. similar [BR07]. similarities [HPPO0].

Similarity [Leh06, LhWX07, ARL01, BPCD07, COS01, Con02, HM08, MBH+02, PDS01, RSS09, YNNW05, hYDN+08, ZZTS09, dGWH01]. similarity-based [RSS09]. similarity/dissimilarity [hYDN+08]. Simple [MO01, Ste04, ACLD03, Bac04, BLMS08, GRO+03, GDV03, Gon07, ILB03, IT03, KS02a, LLW+09, MCF05, SF05, BG00]. simplex [DV02, MCF05]. simplex-annealing [MCF05]. simplified [OYH05, WOC+03]. simulate [LAEL01]. simulated [ADM+06, AB08, CCP04, HPP00, RLP08, WM06, WG02]. Simulating [Fie02]. Simulation [FBGD06, WWL+09, BBHD04, BVW04, BG07, BBN+09, CCD+05, CV09, CHB+05, Dra00, EAA06, EMP07, FHRR07, FEV+09, FPN+05, GS02, GJK00, HN02, HLBN09, ITS05, IM06, IKYM09, JO02, JGVF05, KSY+00, KB09, KEM08, KPR04, Kri09b, LMCD09, LEV+09, MLG04, MMYY07, MVL+05, MLCD01, MST+08, ON07, OBT09, Pin01, PHH+08, SO07, SLO6, SDL07, TYN05, VHR07b, WEE01, XKG+05, YAC+02, YTH+07, ZALMG03, ZWTP+08, ZL09b, ZSK07, OBBS05].

Simulations [FCP+05, MZL08, ATMK03, Ano06c, BWE05, BRDC02, Bi04b, BSJ01, CLP09, CLWL09, CLC09, CCS00, CF06, CPC+00, CEP07, CMD+04, CBH+03, DHF+05, DLRZ09, DFB09, Der00, DSS03, DWC+03, ESM06, FGR07, FG02, FCP+04a, FAB+00, FC06, FKZ09, GL04a, GLP08, GWM08, GHH07, GS03, Gon07, Haf08, HB09, HGM04, HHHS01, HHH04, HM02, HPL03, HHH02, HRG07].
Hin00, HFSD03, HTKG08, HTSR04, HTN03, HMD06, IC08, JNV08, JCL05, JZD+09, KM002, KFZ03, KMi00, KKC05, KAK+09, KvGH01, KH06, Kri08, Kr003, KBN02, LML+00, LSO04, LGB+09, LM03, LPB03, MB00, MFB04, MN02, MABM09, MBC08, MO09, MG00, NK01, NL07, NIl09, OO06, OR05, PRKP05, PJH+08, PB04, PMB04, PK04, PB02, PNG08, RPMP03, RSER09, RMHK03, SK09, SDL+09, Sch04, SBG+09a, SRW06, SR09, SDM02, VCM01]. simulations [VHR07a, VP09, WL09a, WCF04, WZW+06, XLZ08, YNZ+08, YGLvG06, ZCS04, ZSC05, ZGFL01, ZWS+09, ZWZ09, ZSK07]. simulator [JGVF05, KIM+09, MS04, SO07]. simultaneous [DDVD09]. Singh [JVVK09]. Single [OV03, BG07, CV09, HSF08, IT03, IKYM09, LFZS04, WTKM06, XWL+09, ZvRSC08, Mak08]. single-family [WTKM06]. Single-nucleotide [Mak08]. single-sphere [LFZS04]. Single-step [OV03]. single-walled [XWL+09, ZvRSC08]. singles [IN08, WKYU01, dSVA+09]. singlet [BLO+02, CZ05, CG08, FG03, LS08a, OSA06]. singlet-dioxygen [BLO+02]. singly [HHWG08]. Singular [FPG+06, TBSM09]. Sir [Ano04a]. Site [CJW+09, LLL07, AG00, CFR06, CFS+09, CF04, CFC+08, FPN+05, GJK00, GS+07, HFS+07, HYR06, KSK00, KEO4, KZRO03, MDA08, NL07, NLL+09, PMM06, SS05, SPT+03, SFR07, TDH06, XLZ08]. sites [APG05, BSO06b, BSDM04, CLXC02, CLS+09, FPN+05, FSS00, GDV03, HM02, HN02, HLT+05, MHS06, PPXP01, SEKS09, SLC+09, Tie09, Wou00]. six [GJK00, NL07]. six-site [GJK00, NL07]. sixth [CGB+09]. sizable [CAG07]. size [BSOB05, EL09, HLTLP09, KS02a, KH06, NL06, OBBS05, OV03, YAÇ+02]. sized [SHH07]. Slater [CVVB04, EdlVR+03, GC02, KG+09, RLER04a, VB03]. Slater-type [CVVB04, EdlVR+03, GC02, KG+09, VB03]. slave [FR06]. small [CN03, Che01, CG06, FM00, IME02, IO08, JARM02, KvGH01, Lhe06, LZA02, Oos09, PO03, PBZ00, PDS01, RRS09, RZWS07, SHH07, TYO+02, Van02a, WS02b, ZP03, ZOJ+06, ZW09]. small- [SHH07]. smallest [SR07]. SMART [TTBM09]. SMART-based [TTBM09]. smooth [GP01, KSY+00, PZS04]. smooth-particle [KSY+00]. smooth-permittivity [PZS04]. smoothed [LV08]. smoothing [HPP00, ILB03, WS02a]. snapshot [YNZ+08]. SnCl [RD00]. sodium [FL07, MHS05, YSJ09]. SODOCK [CLH+07]. Soft [yCK+08, ASDP+06, TLK+00, TJE03, TGGP+00]. soft-core [TLK+00, TJE03]. Software [Ano04b, BACJCT01, DV+01, Gly06, JKV+09, CH+05, GBDP05, KB+04, MMP+07, NSU+02, BLM+08]. solar [KS05c]. solid [CFS+08, CCG+09, CMA+08, EGSG00, Ish02, KCS+08, SK05]. solid-state [CMA+08]. Solids [vDSSvA04, JB04]. solubilities [SHH07]. solubility [BBG+04, EDJ+04, KEH+02, LLW+09]. solute [BRL+09, BRLS12, FCP+05, LFZS04, MR04, YL09, ZSK07]. solutes [BL+06, HMS06]. solution [ABWT09, BHW00, BP07, BIBS02, BH03, CPJ00, CCK01, CRSB03, DA01, EK00, ELK+09, FHR07, FG02, GMA04, HHJ03, HMWC03, HSW01, HRR05, HBW00, HBW01, HDO+02, KPR04, Kri08, Kri99b, KBN02, LRI+02.
solution-phase solutions [TDH06]. Solvation [COL01, HHP04, WB04b, WB05, WD04, BCIB05, CRSB03, CCT+03, COL+06, DV02, DHW+00, FOL+04, FBLO08, FZL+06, GS02, GS03, GPN01, GWS+02, HC08, HLMR06, IV04, IvSV08, RP04, Sch00, SDL07, VM02, VP09, XL02, ZFL+05, ZFL+05]. solvation-effect [SDL07]. solvatochromatic [XZ04]. solve [KvGH01, XOW+00, Zho06]. Solvent [BA03, BA04b, SMAdV00, ZP03, ZGFL01, AG03, BHW00, BBHD04, BMLV04, BRLS08, BRLS12, ENM+04, FEVM01, FC06, GZL02, GL04a, GP06, GB04, HHS+05, HN02, JS07a, JZD+09, KIFK07, Krö03, KKS04, Lab08, LRI+02, LFBS07, LS04, LL01, LFR+04, MBC08, MM07, MCM04, MS01, PMBO4, RRZ08, RP07d, SBLK01, STSF02, SHSF05, SL06, TJE03, TSMNG01, Tot04, VBGL+00, WB04a, WB04b, WB05, WWL+09, YTY07, YXZ+04, YL09, ZC09, BA04a, FZL+06]. solvent-accessible [BHW00, BMLV04, HHS+05, TSMNG01]. solvents [GS03, IT03, THHN01]. Solving [FS00b, Hof05, BF04, CCL06, CF04, LMJ02, SATO04]. Some [VE09, FMPS08, JARM02, KCL06, McD08, Rao00a, Sch03, WL04, YLL+09, CMA+08]. sometimes [BE06]. Song [JW12]. Sons [Bi09, Lip00]. source [CSV+07, GCB03]. soybean [TGLL07]. sp [NYK+09]. space [Bie04a, BMTSC01, CSJ01, CvG08, CKT+08, CZA03, GT03, HXLS09, JO02, KF08, LCKL05, LJKL08, Nak02, NA06, OFIK09, PRR+05, PBF07, PBF09, PRSMM02, QNF09, Sch04, THHN01, Van02a, YL06]. spaces [JHPRSM+05, PRSMM02, PRT+07, PRT+08, RSS09]. spacing [ZZvRSC08]. spanning [SN00]. Sparkle [FRS05]. Sparkle/AM1 [FRS05]. Sparse [SSB+03, AGSFAL05, LEK07, RS05, RRS07]. sparsity [JSCH07]. spatial [Bie04a, Bie04b, RP07b]. special [KAK+09]. specialized [Hi05]. species [CFC+08, DR09, GHLK+02, HBM06, KZY09, WG02, YIN03, LGMR05]. Specific [FAR02, LR03a, BS08, HLT+05, Pin01, PRJ02, SFRS01, TGLL07, TST+08, UHH09, WCF00]. specificities [PB06]. specificity [CJW+09, DLRZ09, LLL07]. specified [Fau01]. spectra [Bac09, BACJCT01, CNN07, CG08, GCR01, HKHN08, JARM02, KŠB09, KFD06, LCL+09, MLC01, NRKH02, OBBS05, OKE+02, ŠBL05, SN06, TDI06, WM01, YXZ+04, ZGXX06, ZWTP+08, dGWH01]. Spectral [II02, CVR08, GDSUM+07, LFZS04, NAT+07, NAT07, SMK00, WG02, ZSK07]. spectrometric [KZW+05]. spectroscopic [An06a, FCW06, KCL00, ST06]. spectroscopy [ACM+06, RDM+08, VDM06, WMRW+01, ZPL07]. spectrum [EL09, LMC09, MWL+08, MGLDS00, PRSMM03]. Speeding [KVF+07]. speedup [BYQS03]. sphere [HdMS05, Hds06, HDO6, LFZS04, SFR07]. spherical [BCIB05, ZFL+05]. spheriphane [CS01]. SPICKER [ZS04]. Spin
[Duk01, HYR06, KTM02, LXS08, Van02b, ACM+06, BB08, BACJCT01, CR08, CR09a, DXW08, DPT03, DF04, JSHG07, KRM+02, KRLD09, KK08c, LB08, Mck07a, Mck07b, VCM01]. spin-crossover [KRLD09]. spin-label [VCM01]. Spin-orbit [KTM02, LXS08, CR08, CR09a, DXW08, KRM+02, LB08]. Spinor [PV03]. spins [JD09]. Spiro [HELM09]. spiroquinazolinones [DD08]. spline [ALKH04]. splines [GL04b]. split [EA08]. split-valence [EA08]. splitting [PSDM00]. splittings [HLLN06, SFRS01]. Spontaneous [Sza08]. square [CSB08, LLZL09, Nil09]. square-planar [CSB08]. squares [CSD05, Gol09]. Sr [WD08, SCP08, XB08]. Sr-doped [SCP08]. Src [OO08]. SrFeO [Hua09b]. SrZrO [SM06]. SSB [KVS+06]. st2nmr [PRJ02]. stabilities [ACM+06, CTFC08, GYCZ04, STC+08, WDXS06]. Stability [JD09, Owe05, PHFC04, WSC09, CJST+03, CF06, HB07, HX08, JS07b, JBKO8, OCP02, PGC05, QB05, XFF06, ZXYF09, ZOJ+06, ZM06]. Stabilization [EBDPM00, HYA02]. stabilized [HSF08]. stabilizing [GZ07]. Stable [HDO+02, GDPCPU07, KYFW07, KZY09, KAS+07, Keo04, LMO09, PP08a, PZ04, STC+08]. stable/nonstable [GDPCPU07]. stacked [RRCA08, SB08]. stacking [CM09, DDBP09, HWT03, KKY01, WR0+06]. standard [ASDP+06, CG06, FBDG06, KOFF09, LFS03a, LFS03b, SSS+09, SL04]. standing [KDG+09]. staphylococcal [JS07a]. Starting [VZVG06, BW+02]. state [Ang09, BBI+09, CW09, CSF+08, CHA+07, Chu07, CAG07, CMA+08, HM01, HNF07, HNF12, Hir08, HP05, IM02, JHZ09, KT02, Kri09a, LM01, LZ05a, LDL+09, NTH09, PO03, PSS+04, POJ01, Qua07, SP08, Sen06, SRF08, TH02, TST+08, TY03, TKN+08, WCF02, WHF08, ZHO8, ZOJ+06]. state-correlation [SRE08]. state-specific [TST+08]. states [Ang09, ABBC01b, Bo01, Bou01, CW09, CN07, DHE+03, DF04, EL07, FC06, FDS00, HFS+07, HYR06, HZ09, IR03, KUB07, LS08a, LWX07, LB08, MW09, MLCD01, NBT04a, NBT04b, OASA06, OVO3, PRSM08, Qua01, SB08, SMK00, VW00, WL+07, XZ05, ZL05, ZL07, ZL09b, ZM03, dSA+09, ABBC01a]. static [FROD08, LD02, Mar03, XWL+09]. stationary [SK09]. Statistical [HFS03, PY0A3, DW08, EC06, KOB03, ML00, RK05, SB08]. statistical-thermodynamic [RK05]. step [BYQ03, BCP03, DLO06, KM00, KO06, MK02, Mck07b, OV03, OOS09, ZW09]. step/particle [BYQ03]. stepwise [LLK06, LFS+07, NS08]. Stereodynamics [CML05]. Stereoelectronic [DD08, PBF09]. stereoisomers [PMCG09]. stereoselective [AGI+00, AGI+07]. Stereospecific [PF06]. Steric [PF09, BDW00, XYN+06]. steroids [AGMPRG+08]. sterols [CSU05]. STFs [DBS08]. stiff [ECA06]. stillbene [CJ+02]. STO [AG03, RLRE01, RLRE05]. Stochastic [AG03, Fau01, KEM08, SAu04, AM09, CS01, DHE+05, GdSuM+07, MKT04, ZZ08]. Stoner [SK08]. stool [FK+09]. storage [PR06]. stored [AT02, MBW03]. stored-integral [MBWP03]. Strain [ST01]. strained [ST01]. strand [GAS04, JS07b].
stranded [AZM03]. Strategies
[DBS08, LJS05, YL09, EKB02a, EKB02b, KEB04, Vis02]. strategy
[BME05, CZA03, LLL+08, MCF07, RI08, SMGE08, Wan09, WS02a].

streamlining [VGB08]. strength [DMJV05, FO08, SEKS09], strengths
[RM07]. stretch [Kle03, SDCG02]. stretching [CPDZH08]. strictly
[FMSA06, TT01, TT05]. Strike [Ano06c, WZW+06]. string [Qua04, Qua07].

strong [LC07, PGG06]. strongest [VHRR07b]. strongly [ONHN00].

strontium [RD06]. Structural [CZFH07, EM03a, Kri09b, LWS07, LFR07,
MS03, BCP03, CKR08, CLF+09, ECM+03, GZ07, HYA02, HHP04, KZY09,
Kar06, KPKZ06, LL07, LJS05, NAT07, OFIK09, PK04, QLHL09, SLC+09,
SVV+08, SRB06, XSHC06, XLC08, ZLJS03, ZWP08, CA07b]. structurally
[AGMPRG+08]. Structure [BMTSC01, CDL06, HHVG08, HRR05, HS07b,
ITS05, KCL06, KPR04, MN02, PGC05, PLC08, PHRR08, RG08, SG07a,
AJ03, AGSF+05, BFD02, BS01, BAH+02, BAA07, CCL03, CZB07,
CDGS09, CDS09, CMaGL+04, CJS+03, CN05, CLA+00, CPUGD09,
CSV+07, DP03, DHW+08, DHW+09, Fau01, FL07, FL0D07, FCP+04a,
FL08, FLK+07, GBL+05, GTC06, GGGL07, GdAcV+07, HHJ03, HEP+02,
HNO2, HP05, ILKR09, JCA+02, JLH03, KP05, KFNH08, KHY00, KOFF09,
KBK+01, KBL08, KIFK07, KWK+00, KGD06, LER07, LJKL08, Lee09,
LP06, LZA02, LZ50a, LCS+09, LW06, LOL+08, LYP+08, LDL+09, LR03b,
Loe03, LLL07, MOP+07, MM00, MLL08a, MM02, NK01, NYH02, NCO+05,
OS08, PD02, PSCD+09, PI3+07, PPM05, PR02, PF06, QB05, RPN07,
RI07, RS05, RRS07, SBB+03, SJJ+04, SB01, SCP08, TD08, TT01].

structure [TGD05, Van02a, VHRR07b, WZY04, WMRW+01, WD08, WS07,
XZ04, XYL+09, ZZY07, ZZZ+07, ZZY08, ZLD09, ZX08, vDSSvA04,
vEMK01, vE01, RRA08]. Structure-based [BMTSC01, HS07b, KBK+01].

Structure-breaking [HRR05, VHRR07b]. structure-properties
[CDGS09, CDS09]. structure-property [JLH03, PSCD+09]. structured
[DC02]. Structures [AB00, CTCF08, HXD08, KSO5a, PCMG09, RSSK03,
Ama02a, BK08, BSP06a, BS05, BVR+07, CUSS03, CWWS07, CRSB03,
DW08, DF04, DSB+02, DB02, DJB02, EBAN07, FOL+04, GYCZ04,
GJL+08, GCCV00, HM01, HZ09, Hua09a, Hua09b, IGN03, Kar01,
KAS+07, KKM04, LDO5a, LWK08, LV08, LLXS02, LhWX07, LS05a,
MKGA06, Mas01b, MHT01, PCYD03, PYS05, RIO3, RSER09, RM00, RRS09,
SO07, SHBD05, SWR06, TXZ01b, TXZ01a, TT08, TD06, VVBV02, WS05a,
WB04a, WB05, WDXS06, WS02b, WS07, Wi06, WW07, WM01,
XFP06, XZL08, YIN03, YN05, ZCL09, ZXY03, ZGXX06, ACMA+06, FFL07,
STC+08, UM03, ZXL+04, ZZ09]. studied [AGO+02, CFC+08, DPT03,
HFS+07, KBL08, LML+00, RGP+07, RIL06, Sen06, SRE08]. Studies
[AW12, ZWS+02, AB00, ADM+06, Ama06a, BY06, BPC01, BJO6, BSJ01,
BTMFR08, CBM08, DBS07, EBAN07, FJ08, GYCZ04, GC04, GJK00,
Han01, HSWW00, MJIzY+08, KCL06, KWK+01, KWK+02, Klee02,
KZW+05, LKY+04, LWS07, LDY+08, LJP+07, LF02, LWY+09, LSY02,
MCR08, MK02, MOP+07, MW00, RPNJ07, RZWS07, SGPS09, SS00,
SWBM08, SJJ+04, SLL+04a, SLHW09, SFR07, ST06, TJM+03, TMBM02, TCSM03, VS02, VMA03, VL00, VS08, WLL01, WLLS04, WLL07a, WyLG+09, WLL+03, WXX03, WCL05, WZXY07, WXK08, XLL+02, XKKL03, YIN03, YFR05, YLLW09, YLL+09, YKK09, ZDS+05, ZWL+05, ZZZ+06, ZAT07, ZXY03, ZL05. **studio** [Gan09]. **Studt** [Ano06a]. **Study** [SBL05, YZ06, ZCS04, ABYM08, ASDP+06, Ama02a, Ama02b, ATH+03, AVB00, AZM03, BAL+01, BTF09, BSB05, BSB02, BLO6, BLO+02, BRLS08, BRLS12, Bor03, BBSS06, BGC+09, BBI+09, BZL05, CMLS05, CC07, CFS+08, CUS00, CU01, CUS03, CJS+03, CLFA07, CZFH07, CCCJ09, CJW+09, Che01, CN05, CSB08, CFD03, CFD04, CPUGD09, ČJJPZ08, CMD+04, CG05, CSB+09, DHM+03, DGD+05, DLR+08, DWS+09, Der09, DMC05, EA08, EBL+08, FÄ01a, FL07, FC06, FD03, FO08, FKT+05, FKM+06, FKS+09, GXK09, GHLK+02, GD09, Gog08, GM01, GLRL02, GGGGL05, GD06, GKTSG04, GBBD09, HWFN01, HLLS05, HSF08, HELM09, HSMT04, HM08, HPL03, HK07, HJCP01, HHP04, HLMR06, IB04, IV04, IvSV06, IK09, mJlZsLyL07, JHZ09, JW00, JFG04, Kan07, KWHH07, KF06, KSN01, KIFK07, KS01b, KKKM04]. **study** [KS05c, LD05a, LMK01, LKJ+04, LPJ07, LKW08, LMCD09, Lee09, LZA02, LL01, LZ03, LW04a, LX07, LWX07, LLL+08, LS02, LLLS03, LMMW04, LS08b, LKCO6, LLW02, LKT04, LDT+02a, LB08, LYZ+08, LDD+09, LMRVFH+09, LL07, MWL+08, MGMM07a, MML+06, Mas01a, Mas01b, MDA08, MdC03, MdD08, MH09, MSBS01, MGG06, MH08a, MM02, MJ00, ND04, NTH00, NBTN04a, NBTN04b, NAT07, OO04, OON01, OY01, OY03, OSA06, OS08, OO08, Pac06, PP08a, Pan07, PGNG03, PGRRNC03, PC00, PFR04b, PG04, PHKG07, Pil03, PMPG05, PRSM03, PA05, PAS07, PMM05, PMPM06, PWFS01, PHRR08, PB05, wQZsLyZ02, QT+08, RG02, RAGL09a, RAGL09b, RB01, RRS06, RP04, RD00, RGG08, RUPH06, RR05, SF07, SOOF05, SURG06, SB08, SG07a, SLL+04b, SMK00, SBG09b, SN06, SPT+03, SCG04, SE08, SSS+07]. **study** [SK05, SLRC01, SVV+08, SMV+09, SSBE06, TBG00, gThDjL+01, TD08, TT02, UNHT06, UNM+01, UM03, VHRR07b, WZ04, WC09, WMW+01, WD04, WLX+05, WLLS05, WDS06, WDXS06, WDZS07, WLL+07b, WCO8, WWT08, WZZ+09, WM04, WOC+03, WD08, Wom09, WDX+02, WRBV03, WC08, WJX+08, XYN+06, XBO8, XDS06a, XFF06, WXX08, XKG+05, XPW09, YT03, YT04, YTY07, YXZ+04, YDWS06, YXC+07, YLZ08, YLW+08, YQQH09, YHD+06, ZP03, ZPL07, ZZL04, ZLLS04b, ZLLS04a, ZLLS05, ZLLS06a, ZLLS06b, ZZW+07, ZZL+08, ZZL+09, ZH08, ZYW+09, ZOJ+06, ZNLL07, ZX08, ZTP+08, ZL07, dSVA+09, dRLMS00, LSAS01, NB04]. **studying** [AGI+00, AGI+07, dVB01]. **styrene** [Ama02a, Ama02b, XPW09]. **subspace** [FSS00b, Har04]. **substance** [CCP04]. **substances** [ATH+03]. **substantially** [RK05]. **Substituent** [JWB05, Lee09, PWFS01, BPC01, HMMS09]. **substituents** [PSF+08]. **substituted** [AVB00, BE06, BE07, HM08, HWGB01, LST08, MMMY07, MRS09, OSA06,
Substitution [ZS+07, BS05, JT06, LFBSK07, SOOF05, SSB07, ZWS+02],
substitutional [FSS00]. substitutions [CM09]. substrate
[BMTFR08, LCC09]. subtype [FTLV01]. subunit [OON01]. subunits
[MML+06, PHFC04]. successful [CLA+00]. successive [IR03],
successively [YK08]. suffice [LLW+09]. Sugiura [TKN+08]. suitability
[FMSA06]. suitable [GL04a]. sulfate [ZZW09]. sulfation [CLS+09]. sulfide
[DLR+08, GGGLL05]. sulfonamide [CQ04]. sulfonamide [FCP+04b]. sulfonamide
[BB08, CAGR08, FCP+04b, LWX07, SZW+05, WLPF05, Ell07, PV03, PTC01]. sulfonamide-adapted [FCP+04b]. Symmetry-driven
[PV03]. Symmetry-generation [Ell07]. Synergistic [GS08]. syngas
[YQQH09]. synthase [BBSS06]. synthesis [HLC09, PHR+05, WLL01],
synthetic [NHH05, WG02]. system
[BL00, HELM09, HRBKB03, IS03, KYL03, LHJ+06, LCGA03, LTDTS07, MM03, PGH+04, PRSMM03, Rud05a, YOB+08, ZAT07]. Systematic
[AST06, CS03, KWHH07, Kob03, LSAS01, MV06, PK04, PG04, RS05, WM04,
WZXY07, ZXY08, Dya02, PWFS01, PV07, SY+03, WK01, EA06, LMH+09].

**systems** [AS00, BHW00, BP01, BME05, BJI01a, BWI+02, CN03, CG06, CvG08, CCK01, CMGDA+07, DXW08, DRMD03, Don08, DK01, EGSG00, Egl07, FZL07, Fau01, GLMV09, HT03, JCA+02, JTR05, JG03, KSS08, KKC05, KAK+09, KBL08, Kle02, Kle03, Kri09a, LMJ02, LC09, LLL03, LDG02, MMLC05, MKGA06, MTB09, MM07, MS01, Oos09, RLDI09, RSN+02, Rud05b, Rud05c, SRS07, SS00, SY+03, SVV+05, ST01, TH02, TT08, WWL+09, WNH03, YCY03, YZ04, vdVGDM00].

**T** [BBI+09, Lu09, PFJ+03, ZKZ+07, DLD+02, Ike04, KVS+06], **T-cell** [KVS+06]. **table** [Kau07, Nil09, SRB06]. **tableaux** [SN00]. **tables** [ARL01]. **tabu** [MGJAARC00, SE07, SE08]. **tailoring** [BG03, KKG+09]. **taking** [SN06]. **TaN** [ZHMW09]. **tandem** [UNHYT06]. **target** [FM00]. **tautomeric** [LS08b]. **tautomerism** [YXZ+04]. **tautomerization** [BA03, BA04a, BA04b]. **tautomers** [HHWG08, PG04]. **TCNE** [GYMN07, TD08]. **tCONCOORD** [SD09]. **tCONCOORD-GUI** [SD09]. **TD** [CHA+07, SBI08]. **TD-DFT** [CHA+07, SBI08]. **TDDFT** [SL04]. **TDHF** [QCK01, QCK02]. **Te** [HKHN08, WWS07, HWFN01]. **technique** [COS01, GKH05, KLM+09, SATO04, TS05]. **Techniques** [Woo01, You11, AM06b, DC02, FSM09, KH05, PAT+09, PDS01, VE09, WSM+09, vGGB00].

**Teller** [Kri08, VDM06], **temperature** [FGR07, JS07a, KT02, KGD06, MN02, TD08, XK08]. **temperatures** [KK01b, TK08, WHH+06]. **tempered** [BBP09, CVVB04]. **tempering** [SPT07]. **templated** [ST04]. **tensor** [BZP09, BAA07, RJ07]. **tensors** [CDL06, KRM+02, ZLD09]. **term** [JCHS07, SP05]. **terminal** [KK01a]. **Terms** [Duk01, BMLV04, HP01, LAR+03, RP07a, YZ06]. **ternary** [Don08, MM07]. **territory** [Sha07]. **terr** [Bac09]. **tertiary** [CMLS05, PRJ02, PF06, SO07]. **tessellation** [LJ04, PTC01]. **tessellationless** [Pom04]. **test** [BCF+09, BUMCMR00, BLN01, BE06, CF04, FPM09, KTM02, SBI08, SM03]. **Testing** [CMaGL+04, BG03, PZS04, WWC+04, WWC+05]. **tests** [KSB+02, NGTB03]. **tetraammonium** [CW02]. **tetraanaphthalenes** [CdML06]. **tetrachloride** [DMIN05]. **tetracoordinate** [MMRV07, SRS07, Wann09]. **tetraacyanoethylene** [LH02]. **tetraacyanoethylene-contained** [LH02]. **tetracyclene** [AS06, AS09]. **tetrads** [MHS05]. **tetrahalal** [LSY02, OB09]. **tetrahydroimidazo** [SPG08]. **tetrahydroimidazo** [SPG08]. **tetrahydroxouranylate** [LvSV09]. **tetramer** [RRCA08]. **Tetraoxide** [JW12, SLHW09]. **tetrapeptide** [DSR+07]. **tetrapeptides** [GKTS04]. **Tetrazine** [JW12, SLHW09, XZ04]. **Tetrazino** [JW12, SLHW09]. **Tetrazino-Tetrazine-Tetraoxide** [JW12, SLHW09], **tetrazole** [dSVA+09]. **TGSA** [GRC01, GCD04]. **TGSA-Flex** [GCD04]. **Th** [NOS+07]. their [Bac04, Bac05, Bac07, BWZ08, BHH+09, DVRP+03, FL08, GCD+08, JHMB+09, JHMB+11, Lee09, Owe05, PCMG09, SWM04, SRK+00, WWT08,
YLWL09, ZXL+04, ZWY+09]. them [YNW05]. theorem [Kar01, RLER07]. theoretic [SWZS04]. Theoretical

[Ano06a, AZM03, BY06, BI06, Bor03, BS03, CNN07, CFD03, CFD04, CG08, COMR+04, FJ08, FL07, FDSA00, GYCZ04, GLH+08, HLLS05, HS00, IGL07, IIK09, mJIZyL+08, JW12, KYFW07, KZY09, KSN01, KS05c, LS08a, LH02, LWX07, LDY+08, LLW02, LDT+02a, LDT+02b, LYZ+08, LMRVFH+09, MMLC05, MCK05, MBM+00, NBTN04b, OCP02, OKE+02, PFR04b, wQZsLyZ02, RTG00, RZWS07, SLL+04b, SFR07, ST06, TKS+01, TJM+03, gThDjL+01, VS08, WLL01, WLLS05, WDS06, WDXS06, WDZS07, WLL+07b, WCL05, WJX+08, XFF06, XKKL03, YTY07, YIN03, YFR05, YLW+08, YQHH09, YLWL09, YHD+06, ZLLS04b, ZLLS04a, ZLLS05, ZLLS06a, ZLLS06b, ZZW+07, ZZW+08, ZZW09, ZXY03, ZL07, BGC+09, CN05, DLR+08, GXK09, Ham07, HRKBF03, HLMR06, Kan07, KKMS04, LC07, LD05a, Lee09, LL01, LLKC06, LB08, MM02, MDI04, NTH00, NSB08, Nye07, OON01, PGRRNG03, PC00, PAS07]. theoretical [RAGLL09a, RAGLL09b, RRS06, RP04, RJLR06, SLHW09, UNHYT06, WLZ+07, WSM+08, Wou00, XWXC08, YXZ+04, ZL05, dRLMS00, Li01, NBTN04a, RD00, UNM+01, ZPL07, ZLD09]. theoretically [WS02b]. theories [JHZ09]. Theory

[BBU+05, SH08, WM12, ALTBO6, ASDP+06, ASY01, BC06, CFW08, CR08, Chun07, CKW09, CPML08a, Cui08, CGS3ST06, DPM09, DSR+07, EL07, EKBO2a, FCW06, FZL07, FG02, FII+07, FLGW00, FS04, FLK+07, FZL+06, GM01, Gri03, Gri04, Haf08, HSMTO4, HS07a, Hol05, ION07, IKN08, IN08, JCHS07, KSS08, KWK+01, KWK+02, KK08c, KZW+05, Kut07, LMB08, LF04, LFZS04, LMGR05, LF02, LLZL09, LDL+09, Lu09, MGGMO7a, Mat03, MW09, MA09, MH08b, ML00, NYH02, NUH02, NTH09, OFIK09, OKE+02, PFJ+03, PSF+08, PU09, PA05, QTdG+08, RB01, RDM+08, RZWS07, SH07, SH02, SZT08, SSMM09, SSB07, SW06, TST+08, Tru07, TKN+08, TKH03, WR+06, WB07, WZY04, WMRW+01, WW03, WCHW09, WL00, WCFH02, WHN03, WCL05, XY+06, XBO8, XL02, XPW09, YCXY03, YH09, YW07, YLL+09, ZLL04, ZHO8, Zho06]. theory [ZFL+05, dOMSL01, vGBBO0, vLBBR12, Blo04, BE09, CGMT+08, GGB07a, PFBO5, PMC+08, SG07b, ZSP05, Be09]. theory-based [XL02]. Theozyme [UTH+03]. there [KT02]. thermal

[LZZC09, LLKC06, Lu09, SFRS01, WXK08]. Thermally [ZALMG03]. thermochemical [BT00]. thermochemistry [LLXS02, ZXL+04]. Thermodynamic [NA06, WR07, WFR08, ZWP08, Blo04, BZL05, KS05b, KK01b, LC06, LLZL09, RK05, SY09]. thermodynamical [KZY09]. Thermodynamics

[UNM+01, HFSD03, JMD+02, MH09, NSU+02, PCMG09]. thermoelectric [XK08]. thermostats [MZL08]. these [LL00]. thiamin [LS08b]. thiazoline [XKG+05]. thio [MMMY07, TTB01b]. thio-substituted [MMMY07, TTB01b]. thioacetalization [RUPH06]. thioamide [LKJ+04]. thioamide-containing [LKJ+04]. thioether [SFR07]. thiolate
GVATG03, GGLR00, HFHL06, IN01, JJH01, LLM08, LMGO+09, Li01, LL01, LH02, LB05, LLS03, MT03, MAF+07, Mck07b, OON01, PGG06, PMPGP05, QZZZ03, Rao00a, SL09, TBG00, WL00, WC08, YS00, ZY01, ZH08, BA04a.

Transferability
[CSB+03, TT05, FDM00, KS01a, OSHS03, RSP03, TFZRG01]. Transferable
[WBSR03, HXLS09]. transferase [SFR07]. transferred [GFS05]. transfers
[XKG+05]. Transform [BWP07, HLM05, ON07, QLHL09, TYN05].
transform-based [HLM05]. transformation [PVdJB00].
transformational [CN03]. transformations [WSM+09]. transformed
[Nak02, NA06, vDSSvA04]. Transition
[FKRE08, LMGR06, TH02, ABYM08, ABBC01a, ABBC01b, Ano06a, Bac05, BP03, BS06, Bo01, BRV+07, BM00, BGJ01b, CWWS07, Chu07, DLW06, Dib05, EL07, GHH07, GM01, Hol05, JHZ09, KRM+02, LW07, LD05a, LH02, LGB+09, LW209, LK03, LK04, NR04, PYCD03, Qua01, Qua07, RRFC+03, SK09, SZT08, ST06, TKS+01, WB07, WL09b, YTH01, ZALMG03].
transition-metal [Ano06a, ST06]. transitions
[CZ05, FC06, JW06, OYK+09, SMKM00]. Translation [RLER05].
transmembrane [GAS04, YMT04]. transport
[Ara04, CM09, FCP+04a, FCP+05, KK08c]. treating [MA09]. treatment
[BCF+09, BZL05, CLA+00, CBH+03, HC08, HHHB00, IB04, JB04, KS05b, KCL00, LS08c, MFB04, MR02, MGLL03, RI07, RP02, XL02]. treatments
[CEP07, DWNB01]. tree [GY08]. treecode [DK01]. Trends [SRB06].
triangulation [BHH+09]. triazines [ZX04]. triazolones [WZY04].
tribenzo [GLRL02]. trichloroacetaldehyde [CU01]. tricoordinated
[LTF+07]. trigonal [JHM+09, JHMB+11]. trimmer [LZ03, RRCA08].
trimers [ABYM08, VS02]. trimethylamine [CPDZH08]. trimethylsilyl
[LLKC06]. triosephosphate [AGK03]. tripeptide [VKP+08].
triphosphate [GS04]. triple [PP08a, RPNJ07]. triple-decker [RPNJ07].
triplet [CZ05, CG08, FDSA00, LS08a, OSA06]. tripodal [HA04].
trisaccharide [GBB07]. tRNA [GGT08]. truncated [KK08a]. Truncation
[RRS09, MN02]. Trypan [SRK+00]. Trypsin [JZD+09, CWV+05, MBC08].
Trypsin-ligand [JZD+09]. tryptophan [HLC09, Li01, LL01, MM05]. Tsi
[XFF06]. TTTO [JW12, SLHW09]. tubular [FL07]. Tuczek [Ano06a]. tumor
[WCF04]. tumor-specific [WCF04]. Tuning [JHMB+09, JHMB+11].
tunneling [Chu07, MKT04, RBWH09, SRFS01]. TURBOMOLE [LLL03].
turns [HL08]. Two
[PFB05, Yas08, AMR04, AHK02, BR05, BE09, CVRS08, CCK01, DHF+05, FBG06, FR06, GGP09, GMN07, GGA00, HK08c, JJK+00, CAS+07, KT02, Lai07, LDC+07, LWW+06, Sen06, Stoo5, Van02a, Van02b, YFR05, dSR08].
two- [Lai07]. two-body [FBG06]. two-center [BR05, GGA00].
two-component [Van02a]. two-dimensional [CVR08]. Two-electron
[PFB05, Yas08, FR06, GMN07, GGA00, Lai07].
two-electron/four-centers [GMN07]. two-state [KT02, Sen06]. type
[Bic04a, CJDK09, CVVB04, EdiVR+03, GC02, Grio6, HLC09,
IKN08, KDG +09, Leh06, MY08a, OON01, SDL +09, TW03, TLOG00, VB03, WD08, YXC +07. **Typical** [SMV +09, MLL +08b]. **Tyrosine** [AG00, CLS +09, LRI +02, Li01, LL01, OO08].

U [Han01, CCCJ09, GHLK +02, RL09]. **Ubiquinone** [IN01].**Ubiquitin** [KIFK07]. **UCSF** [PGH +04]. **UF** [Han01]. **UK** [Lip00].**Ulcrogenic** [CMBC08]. **Ultra** [ZHWM09]. **Ultra-incompressible** [ZHWM09]. **Ultrafast** [BR07]. **Ultrasound** [PSS +04, PSMB05]. **Unbiased** [Pul05, SYC08]. **Uncertainty** [SY09]. **Uncorrelated** [PSC +01]. **Understanding** [CAGR08, CDPL09, BRS07, ZZW09, CFER04, HP04]. **Unicorns** [FK07b].

**Unified** [GDPP08, CMGDAC +07]. **Uniform** [HdMdS05, HD06, Rap06]. **Unimolecular** [ML00, FS00b, KZY09, ZZL04]. **Unique** [KT02]. **Unit** [VM07, Yas08].

**Unitary** [KBT03]. **Units** [CXZ +09, FEV +09, HP05, NK01, NL08, PC00, PFC03]. **Universal** [DHW +00, HdMdS05]. **Unorthodox** [KBB09]. **Unphysical** [OV03]. **UNRES** [HXLS09, NCO +05]. **Unrestricted** [YH07]. **Unsaturated** [BS03, KFD06, MTB09, Wan09, ZKZ +07]. **Unusual** [KK08c]. **UO** [IV04, IvSV06, RDM +08]. **Update** [BSK02]. **Updated** [Chu07]. **Updates** [Ano04b, BACJCT01, DvL01, Gly06, JVV09]. **upon** [OFIK09]. **Uracil** [LMGO +09, MSBS01, MHS05]. **Uracil-base** [MHS05]. **Urealy** [IV04]. **Urea** [SK05, AS00, VVS07]. **Ureas** [ESM06]. **Use** [BW1 +02, DW08, Wou00, ALB09, FC06, JNV08, Kli01, MRC03, OCP02, PRK05, PRS04, RCJ02a, RSN +02, Ruv07, SH07, SVT09, VGGMM05, YTH01, YZ04]. **used** [DvG00, ESP04, HdMdS05, HdS06, HD06]. **user** [DPDG05, JKII08]. **uses** [KBB09].

**Using** [CSD04, FSM09, HL08, Kae05, LL07, MO01, OSHS03, QLHL09, SWR06, XSC06, XL08, XOW +00, Adc04, AJ03, ABWT09, AM06b, AS00, BWP07, BMLV04, BVW04, BME05, BGC +09, Bud07, CLWL09, CN03, CSJ01, CL09, CKR08, CLA +00, Chu07, CP08, CP09, CPCR04, CPML08a, CGSdST06, DLL +02, DWN01, DR09, DVP +02, DB06, DIB02, DMJ05, EKO +01, EKB02a, EM03b, FCW06, FMP08, FBGD06, FAB +00, FEV01, FR06, FSFK05, GMA04, GL04b, GdSuM +07, GPSP06, GGLR00, Ha08, HWD03, Han01, HSM04, HMS06, HMS09, HG08, HHP04, I02, IS07, IS03, IT03, IK00, JBGK08, JIK09, JVV09, JTR05, JFG04, JSG07, KRM +02, KKO +09, KM00, KKH +04, KK08c, KOFF09, Klem02, Kle03, KBT03, KKS04, Lab08, LCKL05, LCC09, LZ05a, LLL +08, LZZC09, LS05a, LZ05b, LS05, LW04, MWL +08, MT03, MML05, MKT04]. **using** [MV06, MBP09, MOP +07, MTE04, MRS09, MRS +07, NCO +05, NINAT +07, OFB08, OEK +02, PMB04, PS00a, PAT +09, PP08b, PSD01, PZS04, PSS +04, RI07, RIO8, RPM01, RC08, RON02, SDL +09, SPGS08, SSB +03, Sch00, SRE03, SBG +09a, SY09, SPT07, SMV +09, TP01a, Tiese09, TCSM03, UBDP04, VSW +03, Van02a, WLZ +07, WL00, WEE01, WO02, WOC +03.
v [Lip06, ZZW09, GB03, Kri09b, PFC03, TD08]. vacancy [ZMH+09].

vacuum [BISB02]. Valence [LW07, SH08, Tru07, WM12, Bic09, BLT03, Cns08, EA08, HELM09, HS07a, May07, MG00, PRSMV08, SWZS04, SMZW05, SSMW09, SSW+07, VBGL+00, WMRW+01, WJ00, dSVA+09, vLBBR12]. valency [Lip00, ZZW09, GBJ03, Kri09b, PFC03, TD08].

validation [BAA07, VCM01, AGI+00, DGD+05, JJB02, JAC05, MSR04, SRB06, APG05, HZ06b, NGTB03]. valinamide [HJCP01].

value [FPG+06, TBSM09]. values [OS06, PMPG05]. vanadium [PV07, Tie09]. vapor [PHJ+08, UNM+01].

variable [CFS+09, GS08, WHRG08]. variables [SWR06]. variance [Blo04, LRWG03]. variate [LR06]. Variation [AAP00, NAT07, PGG06, Rao00a, Vya01]. Variational [MR02, AB09, Chu07, GY06, HdmS05, Hsd06, HD06, RS07a, RS07b]. Variations [TGGP+00]. variety [SBL05]. various [BP07, HMM09, IT03, Kr03, KS01b, MLL+08b, PP08a, PFJ+03, PPM05, RR05, WHH+06, ZCL09]. varying [CC09].

VAP [Haf08]. VBSCF [vLBBR12]. VCH [Sta00]. VDD [GHBB04, GHBB04]. vector [CLXC02, CLS+09, HL08, LCC09, LJZ+07, QHL09, YMT04]. vectorizing [SO07]. vectors [BWI+02]. versatile [KF08, TDMSD+08]. version [HBBD04]. versions [Sto05]. versus [ABY08, ALCO8, BSch07, BB08, JS07b, JBKG08, LST08, LT08, PSM05, Van02b]. Vertical [PRSM03, SA07, CG08, LWX07, LFEAL06, SLRC01, TK+01]. VI [HP05].

via [BA03, BA04a, Bou01, BR500, BR501, CGB07, CAG07, DFG09, Hu09a, JP09, KSB+02, KRL09, LMO09, SMM+08, SG01, ZPL07]. Viability [K01b]. viable [LMM05]. Vitalizer [Gra07]. vibrating [Yos02].

vibration [CCL06, LSY02, ZWP+04]. Vibrational [BP07, CLP+05, LC09, NR04, WB07, BRV+07, DB07, GBDP05, Gra07, Han01, Hnr08, JARM02, LMB08, LN01, MR02, NRKH02, NAT07, PZW+04, Tor02, WM04, WM01]. vibrations [CPDZH08, DR09, KCL00, vE01]. vibronic [TP01b]. view [CSJD04, Jac09, JMD+02, MGCA07]. VIII [EBD+01]. vinyl [YYW07].

vinylphosphine [MGLD00]. viridis [IN01, OON01]. virtual [GS05, KSM05, LZ05b, PRD08, YOB+08]. virus [AJNG01, DLR209, KCL06]. viscosity [ZP03]. Visualization [MMP+07, RP07b, AR01, KYL03, PGH+04]. Visually [SD09]. VMD [Pra01]. VMFCI [CCL06]. VO [PV07]. voltammetry [KJP+07]. Volume [Sta00, BVW04, Lab08, LFSB03a, LFSB03b, Muc01, QNF09].

volume-preserving [QNF09]. volumes [BH1+09, Rao00b, SBLK01]. Voronoi [GHBB04, MVLG06, SBLK01]. VPI [KCL06]. VPP700 [KSY+00]. Vpu [KF08]. vs [CZ+09, LLKC06, MA05, SCS04, Wib04].
REFERENCES

Z [CRC+08, PWFS01]. zeolites [LTV08, SDCG02, TLOG00]. zeolitic [Tie09]. Zerner [Ano00]. zero [RKA+09]. zero-flux [RKA+09]. zeta [CMJ08]. Zhang [Ano06c]. Zhi [Ano06c]. Zhi-Xiang [Ano06c]. Zinc [CFS+08, BSDM04, ECM+03, JT06, JT08, KZRO03, RGP+07, SFR07, SCF+09, SDM02]. zinc-[SDM02]. Zintl [XB08, ALC08]. zirconocene [LHP01]. Zn [BTP09, GSP06, BBI+09, ESM06, FO08, GPK05, ROG00, TGGP+00, TFZRG01]. Zn-biomimetic [FO08]. ZnO [HSF08]. ZnX [WWS07]. Zori [AGSFA+05]. ZPE [MGLDS00]. ZPVA [QCK01, QCK02]. zwitterionic [ROG00]. zwitterions [KLB03]. zymogen [PDP02]. ZZ [CRC+08].

References


REFERENCES


[ABBC01b] Josep Maria Anglada, Emili Besalú, Josep Maria Bofill, and Ramon Crehuet. On the quadratic reaction path evaluated in a reduced potential energy surface model and the problem to locate transition states. *Journal of Computational Chemistry*, 22(4):387–406, March 2001. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [Qua01], reply [ABBC01b], and erratum [ABBC01a].


Addicoat:2008:AVD


Angyan:2003:OTO


Allinger:2003:AEC


Atanasov:2006:DMC


Allinger:2000:VWE

REFERENCES


REFERENCES


Dominic R. Alfonso and Kenneth D. Jordan. A flexible nudged elastic band program for optimization of minimum energy

**Abrahao-Junior:2001:CAH**


**Akama:2007:IDC**


**Agrafiotis:2001:MSC**


**Allen:2009:GMG**


**Alemany:2008:RCE**


REFERENCES

Anonymous:2001:CBC

Anonymous:2001:NSJ

Anonymous:2004:PNSa

Anonymous:2004:PNSb

Anonymous:2005:A

Anonymous:2005:EDS

Anonymous:2006:EFS
REFERENCES


**Anonymous:2006:EMC**


**Anonymous:2006:EZX**


**Antony:2005:CTC**


**Aragon:2004:PBE**


**Agraﬁotis:2001:MSV**

[ARL01] Dimitris K. Agraﬁotis, Dmitrii N. Rassokhin, and Victor S. Lobanov. Multidimensional scaling and visualization of large

**Ayala:2000:ECL**


**Aleksandrov:2006:TMC**


**Aleksandrov:2009:MMM**


**Alves-Santos:2006:ASD**


**Autschbach:2002:DRE**

Altun:2006:SQM


Alexeev:2007:PDD


Arulmozhiraja:2001:BRI


Ahlrichs:2002:ELA


Autenrieth:2004:CFF


Aquino:2003:AOS


REFERENCES


[BAA07] Bård Buttingsrud, Bjørn K. Alsberg, and Per-Olof Åstrand. Validation of critical points in the electron density as descriptors by building quantitative structure–property relationships


REFERENCES

[Bultinck:2002:GPD]

[Balucani:2001:GPD]

[Banerjee:2005:ECA]

[Binning:2008:HSV]

[Banks:2005:IMP]
REFERENCES

Belmares:2004:HHS


Basdevant:2004:SIS


Bucinsky:2009:REG


Brooks:2009:CBS


Bonomi:2009:REB

REFERENCES

1615–1621, August 2009. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


[BBSS06]


[Brown:2006:SDG]


[Barone:2009:RET]


[Benzi:2005:BCF]


[Berente:2007:CEE]
REFERENCES


1783–1789, August 2007. CODEN JCCCHD. ISSN 0192-8651 (print), 1096-987X (electronic).

**Bohm:2009:ITF**


**Ball:2002:ENA**


**Beran:2003:ICE**


**Boschitsch:2004:HBE**


**Boschitsch:2007:NOB**


**Brooks:2007:LE**


Bordner:2003:BES

Brown:2003:CWN

Busa:2009:ETM

Bader:2007:ECB

Baker:2000:AMF

Bharatam:2006:TSE
REFERENCES


REFERENCES


REFERENCES

Bobrowski:2002:ISM


Blondel:2004:EVF


Bochicchio:2003:DAV


Bosque:2000:PSP


Beck:2007:HRA


Bessac:2008:DMR

REFERENCES


[Bras:2008:MSF]

[BMTR08] Natércia F. Brás, Sara A. Moura-Tamames, Pedro A. Fernandes, and Maria J. Ramos. Mechanistic studies on the formation of glycosidase-substrate and glycosidase-inhibitor cova-
REFERENCES


[**Budin:2001:SBL**]


[**Bofill:2001:RCQ**]


[**Borosky:2003:TSC**]


[**Bour:2000:CHF**]


[**Bour:2001:CRO**]

REFERENCES


REFERENCES


REFERENCES

JCCDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [BRLS12].


[BRV+07] Vladimir I. Bolshakov, Vladimir V. Rossikhin, Eugene O. Voronkov, Sergiy I. Okovytyy, and Jerzy Leszczynski. The

**Betancourt:2001:FNH**


**Brana:2003:TAM**


**Bindewald:2005:SFD**


**Blomberg:2006:QCA**


**Brylinski:2008:QDL**

REFERENCES

[BSB05] A. Patrícia Bento, Miquel Solà, and F. Matthias Bickelhaupt. Ab initio and DFT benchmark study for nucleophilic substitution at carbon ($S_N2@C$) and silicon ($S_N2@Si$). Journal of Computational Chemistry, 26(14):1497–1504, November 15, 2005. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES 122

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Benkova:2005:RSP


Beke:2006:TRD


Bhat:2006:CAC


Benassi:2000:CBS


Bastard:2003:DMF


Barman:2009:IMM


REFERENCES


REFERENCES

*Burd:2005:HPA*


*Barone:2009:HMD*


*Curco:2004:PSM*


*Curco:2007:CGP*


*Curco:2007:CTM*

Chatfield:2003:MDC


Conte:2007:DEF


Contreras:2008:UTS


Carpenter:2002:CPC


Chang:2008:EEC


Curutchet:2003:EDM


REFERENCES


REFERENCES


Cuesta:2006:DT

Cuesta:2009:URC

Carbo-Dorca:2009:NQSb

Cordomi:2007:EDT

Chuev:2004:WAS

Chocholoušová:2006:BAR
Jana Chocholoušová and Michael Feig. Balancing an accurate representation of the molecular surface in generalized Born formalisms with integrator stability in molecular dynamics simu-


REFERENCES


REFERENCES


REFERENCES


Chipot:2003:RDC


Chrocker:2005:MAP


Cramariuc:2009:IDP


Chuang:2007:CRC


Chen:2005:ATA


Chen:2009:PIM

REFERENCES


Calaminici:2002:MLF


Condic-Jurkic:2008:MAB


Chen:2003:SSS


Cheng:2009:SSC


Cramer:2001:WAE


REFERENCES


REFERENCES

Cacelli:2009:FFM


Chang:2009:ISV


Cao:2009:RDP


Cai:2002:SVM


Chen:2009:ACP


Chen:2009:MSA

[CLZX09] Weiyang Chen, Bo Liao, Wen Zhu, and Xuyu Xiang. Multiple sequence alignment algorithm based on a dispersion graph and


Corzana:2004:HSL


Cruz-Monteagudo:2007:CCD


Camiletti:2008:GBS


Campomanes:2005:SBR


Carlsson:2003:IPE

Peter Carlsson and Lennart Nilsson. Improved precision and efficiency of free energy calculations for small systems using λ-scaled atomic masses and separating conformational and


REFERENCES

Constans:2002:LSA

[Con02] Pere Constans. Linear scaling approaches to quantum macro-

Chae:2001:FMS


Clarke:2008:TAP


Clarke:2009:IAP


Chun:2000:MDM


Chandra:2008:BSC


**Castano:2002:RBB**


**Carballeira:2000:IIG**


**Carballeira:2001:RAE**


**Ceccarelli:2003:IFF**


**Csontos:2008:CWP**


REFERENCES


REFERENCES


REFERENCES


REFERENCES

Cournia:2005:MMF

Crawford:2007:POS

Cui:2008:SSE
Yan-Hong Cui, Wei Quan Tian, Ji-Kang Feng, and De-Li Chen. Structures, stabilities, electronic, and optical properties of C_{64} fullerene isomers, anions (C and C_{64}^{4-}), metallofullerene Sc\textsubscript{2}@C_{64}, and Sc\textsubscript{2}C\textsubscript{2}@C_{64}. *Journal of Computational Chemistry*, 29(16):2623–2630, December 2008. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chandra:2001:ROR

Cullen:2004:PHF
REFERENCES


[CVR08] Riccardo Chelli, Victor V. Volkov, and Roberto Righini. Retrieval of spectral and dynamic properties from two-dimensional infrared pump-probe experiments. *Journal of
REFERENCES


**Chong:2004:ETS**


**Chaumont:2002:MQT**


**Cho:2005:MDH**


**Cheng:2007:ESC**


**Camacho:2009:ISM**

REFERENCES

Chen:2009:EMI


Chen:2009:PRW


Chen:2013:EPR


Chen:2002:CIS


Cao:2005:CAS


Curco:2003:EFS

[CZA03] David Curcó, David Zanuy, and Carlos Alemán. EVEBAT: a fast strategy for the examination of the empty space in poly-

**Call:2007:GMS**


**Chen:2007:SEO**


**Delgado:2001:PID**


**Dyrka:2008:IFT**


**Djurdevic:2006:IPF**

REFERENCES


REFERENCES

April 30, 2008. CODEN JCCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


**Derreumaux:2000:PHH**


**Derosa:2009:CSD**


**Deeth:2004:PND**


**Darowicki:2006:JTF**


**Dronskowski:2008:F**


**Delalande:2009:CMA**

REFERENCES


Deeth:2005:DIL


DeJong:2005:OAE


Davies:2002:PRM


Donchev:2008:APG


deGelder:2001:GES

Darian:2005:EAI


Das:2003:EEG


Dolney:2000:USM


Du:2007:PRD


Du:2008:MFT

Du:2009:FBQ


Dibble:2005:CXT


Dinner:2000:LDP


Donnini:2004:CAP


Doruker:2002:DLP


Davis:2008:MMP


REFERENCES


REFERENCES

Dixon:2005:QUS

Das:2003:PHM

Dobrogorskaia-Mereau:2005:QCM

Ding:2008:EBF

deOliveira:2001:DHF
REFERENCES


[DPM09] Michael Devereux, Paul L. A. Popelier, and Iain M. McLay. Toward an ab initio fragment database for bioisosterism: Dependence of QCT properties on level of theory, conformation, and chemical environment. Journal of Computational Chem-


[DelCarmenMichelini:2004:ETA] Maria Del Carmen Michelini, Nino Russo, Mohammad Esmail Alikhani, and Bernard Silvi. Energetic and topological analysis of the reaction of Mo and Mo2 with NH3, C2H2, and

[DRAS05] Maria Del Carmen Michelini, Nino Russo, Mohammad Esmail Alikhani, and Bernard Silvi. Energetic and topological analyses of the oxidation reaction between Mo$_n$ ($n = 1, 2$) and N$_2$O. *Journal of Computational Chemistry*, 26(12):1284–1293, September 2005. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


Dennis:2002:SSO


deViterbo:2001:ANN


Damm:2000:RPF


Dijkstra:2001:SNU


DeProft:2002:ACD


DeProft:2003:HPE

REFERENCES


Echenique:2006:DSA


Echenique:2008:EMC


Exner:2004:EFM


Eom:2007:CGP


Ewig:2001:DCI

REFERENCES

El-Bergmi:2000:SNB


Evarestov:2008:FPD


Echenique:2006:EFE


Echenique:2006:QMC


Elstner:2003:MZB


Estrada:2004:QCD

[EDAJ04] Ernesto Estrada, Eduardo J. Delgado, Joel B. Alderete, and Gonzalo A. Jaña. Quantum-connectivity descriptors in mod-
REFERENCES


1. Exner:2002:PRSb


2. Endo:2001:AXX


5. Evarestov:2009:AEL


Frank Eckert, Ivo Leito, Ivari Kaljurand, Agnes Kütt, Andreas Klamt, and Michael Diedenhofen. Prediction of acidity

**Ellzey:2007:FGT**


**English:2003:SDP**


**Exner:2003:IQP**


**Eslami:2007:MDS**


**Eyal:2004:ISA**


**Elezgaray:2000:MDP**

Estiu:2006:QMM

El-Sherbiny:2004:ERP

Estrada:2007:PSN

Ferenczy:2001:II

Frenking:2001:EP

Field:2000:DLM
Martin J. Field, Marc Albe, Céline Bret, Flavien Proust-De Martin, and Aline Thomas. The dynamo library for molecular simulations using hybrid quantum mechanical and molecular


REFERENCES


Freeman:2003:CSC


Fradera:2000:ATW


Fores:2000:TCI


Friedrichs:2009:AMD


Fogolari:2001:MMD

REFERENCES


[FHF+01] Shuhei Fukawa, Masahiko Hada, Ryoichi Fukuda, Shinji Tanaka, and Hiroshi Nakatsuji. Relativistic effects and the halogen dependencies in the $^{13}$C chemical shifts of CH$_{4-n}$In$_n$, CH$_{4-n}$Br$_n$, CCl$_{4-n}$I$_n$, and CBr$_{4-n}$I$_n$ ($n = 0–4$). *Journal of Computational Chemistry, 22*(5):528–536, April 15, 2001.


REFERENCES

2006. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fukuzawa:2007:II

Fritsch:2008:TMD

Futera:2009:IPS

Fukuzawa:2005:IQM

Frickenhaus:2009:EES
Stephan Frickenhaus, Srinivasaraghavan Kannan, and Martin Zacharias. Efficient evaluation of sampling quality of molecular dynamics simulations by clustering of dihedral torsion angles and Sammon mapping. *Journal of Computational Chemi*
REFERENCES


[Ferrante:2007:TSI]

[Flocke:2008:EEI]

[Feldgus:2000:NRT]

[Frenking:2007:ESC]

[Ferro:2007:MES]

[Foloppe:2000:AAE]
Nicolas Foloppe and Alexander D. MacKerell, Jr. All-atom empirical force field for nucleic acids: I. Parameter optimiza-
REFERENCES

Flores-Moreno:2006:HNE


Feixas:2008:PSA


Fornili:2006:SSL


Fuchs:2006:NMP


Fukaya:2004:DGC

Frison:2008:CSS


Fedorov:2004:NHP


Feig:2004:PCG


Fiorentino:2006:SVD


Fujimoto:2005:MDS

Fossgård:2006:SSM


Frenking:2000:F


Fuhrmann:2009:NMG


Ferrero:2008:CSP


Freire:2005:MLC


Forester:1998:SRR


REFERENCES

Fajer:2009:UMF


Fuster:2000:DSS


Filizola:2001:GPP


Fias:2008:MDI


Fischer:2007:IBC


Fu:2006:CMT

Ke-Xiang Fu, Quan Zhu, Xiang-Yuan Li, Zhen Gong, Jian-Yi Ma, and Rong-Xing He. Continuous medium theory for


REFERENCES


Gromiha:2004:NNB


Greene:2002:ICE


Guvench:2004:EAA


Gould:2007:CIQ


Grybos:2009:INM


Gohaud:2005:NPS

Neil Gohaud, Didier Begue, Clovis Darrigan, and Claude Pouchan. New parallel software (\texttt{PAnhar}) for anharmonic vibrational calculations: Application to \((\text{CH}_3\text{Li})_2\). Journal of
REFERENCES


REFERENCES


Garcia-Cruz:2000:DMM


Girones:2004:TFE


Grazioso:2008:ANA


Gallegos:2005:MPD


Gonzalez:2006:PCM

REFERENCES


REFERENCES

Glättli:2003:NAD


Galván:2008:IEN


Genoni:2005:OVO


Goette:2009:ACF


Gill:2000:RET


González:2007:AERa

REFERENCES


REFERENCES

Gresh:2004:IIE


Gallicchio:2004:AAI


Gillilan:2004:ODP


Georgiev:2008:MDE


Geng:2008:TER


REFERENCES


Galvan:2004:NML


Gogtas:2008:TDQ


Golmohammadi:2009:POW


Gonnet:2007:SAA


Goraczko:2001:MMF


Gianese:2006:CPI

REFERENCES

Gresh:2005:RZI

Grant:2001:SPF

Gourlaouen:2006:RGM
Christophe Gourlaouen, Jean-Philip Piquemal, Trond Saue, and Olivier Parisel. Revisiting the geometry of \( nd^{10}(n+1)s^0 \) \([\text{M(H}_2\text{O)]}^p+\) complexes using four-component relativistic DFT calculations and scalar relativistic correlated CSOV energy decompositions (\( M^p+ = \text{Cu}^+, \text{Zn}^{2+}, \text{Ag}^+, \text{Cd}^{2+}, \text{Au}^+, \text{Hg}^{2+} \)). *Journal of Computational Chemistry*, 27(2):142–156, January 30, 2006. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gillespie:2007:EGL

Grafton:2007:VFW
Girones:2001:TMS


Grimme:2003:ITO


Grimme:2004:ADV


Grimme:2006:SGT


Garavelli:2003:SAI


Goncalves:2002:NAF


[GSB09] Adrià Gil, Mariona Sodupe, and Juan Bertran. Influence of ionization on the conformational preferences of peptide models. Ramachandran surfaces of N-formyl-glycine amide and
REFERENCES


REFERENCES

Gu:2007:IGQ


Gooding:2000:FPQ


Gao:2008:CQM


Guvench:2002:AFA


Gao:2009:TSF


Gregersen:2006:CSI

Brent A. Gregersen and Darrin M. York. A charge-scaling implementation of the variational electrostatic projection


Grosdidier:2009:BDP


Howard:2004:ICH


Hafner:2008:ISM


Hamacher:2007:ITM


Han:2001:DFS


Harrison:2004:KSA

Hamaneh:2009:RPH


Harvey:2006:QMM


Holst:2000:AMF


Holst:2001:EAM


Haberthür:2008:FFA


Haiduke:2006:ARAAb

Roberto L. A. Haiduke and Albérico B. F. Da Silva. Accurate relativistic adapted Gaussian basis sets for cesium through radon without variational prolapse and to be used with both uniform sphere and Gaussian nucleus models. *Journal of Computational Chemistry*, 27(16):1970–1979, December 2006. CO-
DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


REFERENCES


Hirama:2003:PMH


Heine:2007:CIM


Hinsen:2000:MMT


Hirao:2008:RBO


Hudaky:2001:PMX


Hou:2007:DSD

REFERENCES


REFERENCES

Han:2001:AMS

Hu:2008:USV

Huang:2009:MDS

Hofto:2009:IA

Han:2006:DCM

He:2005:TSR
Hong-Qing He, Jing-Yao Liu, Ze-Sheng Li, and Chia-Chung Sun. Theoretical study for the reaction of CH$_3$OCl with Cl


Huo:2002:CAS


Hemmateenejad:2009:AMA


Huey:2007:SFE


Hemmateenejad:2006:APB


Haberthur:2003:EEE


Higo:2002:HSH

[HN02] Junichi Higo and Masayoshi Nakasako. Hydration structure of human lysozyme investigated by molecular dynamics simu-


REFERENCES

Holthausen:2005:BAD


Hassinen:2001:NET


Hill:2004:RSP


Hudaky:2005:TDD


Hernandes:2003:CSL


Hart:2000:ESB

REFERENCES


Hirsch:2002:IRM


Hill:2008:GFE


Hermida-Ramon:2003:IIP


Hermida-Ramon:2007:BSH


Hofer:2005:SBE


Headley:2000:TAF

Allan D. Headley and Stephen D. Starnes. Theoretical analysis of fluoroglycine conformers. Journal of Computational Chem-


**REFERENCES**


[Hg01] Junichi Higo, Yasunobu Sugimoto, Katsuzo Wakabayashi, and Haruki Nakamura. Collective motions of myosin head derived
REFERENCES

Hong:2000:CED


Hopkins:2003:MAI


Harman:2005:CDD


Hnizdo:2008:ECC


REFERENCES


[HXD08] Ning He, Hong-Bin Xie, and Yi-Hong Ding. Structures and stability of lithium monosilicide clusters SiLi$_n$ ($n = 4$–16): What is the maximum number, magic number, and core number for lithium coordination to silicon? *Journal of Computational Chemistry*, 29(11):1850–1858, August 2008. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

REFERENCES


Helal:2002:ICS

[HYA02] Mustafa R. Helal, Yaser A. Yousef, and Akef T. Afaneh. Ab initio calculations of the stabilization energies of the conformational and the structural isomers of \( \text{C}_3\text{H}_7\text{X} \) where \( \text{X} = \text{F}, \text{Cl}, \) and \( \text{Br} \). *Journal of Computational Chemistry*, 23(10):966–976, July 30, 2002. CODEN JCCCHD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yao:2008:ASD


Herrmann:2006:SSP


Hatano:2005:CMO


Huang:2006:IKBa

REFERENCES


REFERENCES


Irbac:2006:PMC


Ida:2002:ESS


Ito:2001:RPE


Imamura:2008:EDA


Inada:2008:ENB


Imamura:2007:DCE

[ION07] Yutaka Imamura, Takao Otsuka, and Hiromi Nakai. Description of core excitations by time-dependent density functional theory with local density approximation, generalized gradient approximation, meta-generalized gradient approximation, and

[Ishimura:2006:NPA]


[Ishimura:2007:NPA]


[Ivanic:2003:MMG]


[Ishida:2003:LIS]


[Inaba:2007:DPD]


[Ishida:2002:ACE]

Kazuhiro Ishida. Accompanying coordinate expansion formulas derived with the solid harmonic gradient. *Journal of Com-

Ishida:2003:MIG


Ishida:2004:AFA


Iwaoka:2003:SFF


Inaba:2005:AED


Intharathep:2005:SDH


Intharathep:2006:IQM

Pathumwadee Intharathep, Anan Tongraar, and Kritsana Sagarik. Ab initio QM/MM dynamics of H_3O^+ in water. Jour-
REFERENCES

Infante:2004:QMS


Infante:2006:QMS


Izrailev:2006:DGH


Jacobsen:2009:CBV


Jiang:2002:CPE


Jug:2004:MTC

Janetzko:2008:BDD


Janetzk:2008:BDD

Jakalian:2000:FEG


Jakalian:2000:FEG

Jacquemin:2002:IAD


Jacquemin:2002:IAD

Jurecka:2007:DFT


Jureck:2007:DFT

Jha:2005:FFV

Jin:2009:SBS


Jin:2006:RMC


Jung:2004:CMF


Jug:2003:BEM


Jug:2000:MPT


Johnston:2005:FBD

REFERENCES

2005. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jimenez-Halla:2009:TAT


Jimenez-Halla:2011:ETA


Ju:2009:GDT


Jiang:2009:PPF

REFERENCES

Jakalian:2002:FEG


Jongejan:2001:DHT


Jenkins:2000:BSC


Jo:2008:CGW


Johansson:2008:CPM


Jena:2008:RHA

REFERENCES

98–107, January 15, 2008. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


Jug:2000:MSL


Jang:2006:MPC


Jorgensen:2012:LEC


Ju:2005:SEH


Jiao:2009:TLB


Kikugawa:2009:AMS

Gota Kikugawa, Rossen Apostolov, Narutoshi Kamiya, Makoto Taiji, Ryutaro Himeno, Haruki Nakamura, and Ya-


REFERENCES


REFERENCES

Kover:2009:CNT


Kuttel:2002:CSS


Koslowski:2003:IGM


Kraka:2001:PDP


Kristyan:2001:FAC

Kim:2008:PDS


Kirtman:2000:ETE


Ke:2006:SVC


Kang:2009:LAS


Kony:2002:IOA


Keil:2004:PRS

REFERENCES

Klamt:2002:PAS

Kovalyov:2008:SSP

Kleppeis:2002:IPH

Ko:2002:RCL

Kleppeis:2003:PST

Kruger:2008:ECS
Karney:2005:MCP


Knippenberg:2006:GFS


Katagiri:2008:IPS


Kaminski:2003:CIM


Kairys:2002:EDM


Kurtulus:2006:ESC

Yasemin Kurtulus, Michael Gilleßen, and Richard Dronskowski. Electronic structure, chemical bonding, and finite-temperature magnetic properties of full Heusler alloys. *Jour-
REFERENCES


Kiyota:2009:MQM


Khandogin:2000:ESP


Komeiji:2007:CPE


Komeiji:2009:FMO


Kim:2007:CVM

Kyoung Hoon Kim, Jaehoon Jung, Bo Keun Park, Young-Kyu Han, and Joon T. Park. Cyclic voltammetry modeling, geometries, and electronic properties for metallofullerene complexes with $\mu_3$-$\eta^2$: $\eta^2$: $\eta^2$-C$_{60}$ bonding mode. *Journal of Computational Chemistry*, 28(6):1100–1106, April 30, 2007. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
REFERENCES


[KK08c] Woo Youn Kim and Kwang S. Kim. Carbon nanotube, graphene, nanowire, and molecule-based electron and spin transport phenomena using the nonequilibrium Green’s function method at the level of first principles theory. *Journal of
REFERENCES


**Kang:2009:CPM**


**Khan:2005:SPM**


**Kavathekar:2009:WWI**


**Kim:2007:EEG**


**Kim:2008:RMD**

<table>
<thead>
<tr>
<th>Reference</th>
<th>Authors</th>
<th>Title</th>
<th>Journal</th>
<th>Volume</th>
<th>Pages</th>
<th>Year</th>
</tr>
</thead>
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<tr>
<td>[Kle03]</td>
<td>Roger A. Klein</td>
<td>Hydrogen bonding in diols and binary diol-water systems investigated using DFT methods. II. Calculated</td>
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</tr>
</tbody>
</table>

**Kim:2004:PPP**


**Kliesch:2001:EEP**


**Korchoiewiec:2009:ECT**


**Kazmierkiewicz:2002:EBR**


**Kawata:2000:CEC**

Kawata, Masaaki and Masuhiro Mikami. Computationally efficient canonical molecular dynamics simulations by using a multiple time-step integrator algorithm combined with the particle mesh Ewald method and with the fast multipole

Kegerreis:2007:OMC


Kent:2007:EAF


Kalat:2002:QPG


Khoroshun:2007:ER


Kawamura:2004:HAC

REFERENCES


REFERENCES

Karamertzanis:2005:ICS


Kritayakornupong:2004:SDC


Kuta:2006:PDM


Kritayakornupong:2008:JTE


Kristyan:2009:IPT


Kritayakornupong:2009:SDP

Kri09b Chinapong Kritayakornupong. Structural and dynamical properties of the V$^{3+}$ ion in dilute aqueous solution: an ab

### Kepenekian:2009:EFN


### Kaupp:2002:CET


### Krol:2003:CVI


### Kedzierski:2001:ATA


### Krüger:2001:DSH

REFERENCES


Kim:2008:APL


Kaminski:2002:DPF


Kaminsky:2009:MDR


Kedzierski:2000:NAN


Kontoyianni:2005:ELR


Kobayashi:2001:TSE

Kerb:2008:ASL


Klopper:2001:EIB


Kamiya:2003:ANM


Kholmurodov:2000:SPM


Klimov:2002:TUM


Karipidis:2008:DEN

Katritch:2003:INM


Kleinschmidt:2002:SOC


Kloppmann:2007:EDE


Kutzelnigg:2007:EWL


Koehler:2000:DSL


Kutzner:2007:SPG

REFERENCES


**Kim:2001:DFT**


**Kim:2002:EDF**

Chang Kon Kim, Jongok Won, Hoon Sik Kim, Yong Soo Kang, Hong Guang Li, and Chan Kyung Kim. Erratum: Density functional theory studies on the dissociation energies of metallic salts: Relationship between lattice and dissociation energies. *Journal of Computational Chemistry*, 23(5):584, April 15, 2002. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [KWK+01].

**Kan:2007:TIP**


**Kozhin:2003:NVS**


**Kirschner:2008:GGB**

Karl N. Kirschner, Austin B. Yongye, Sarah M. Tschampel, Jorge González-Outletiño, Charlisa R. Daniels, B. Lachele Foley, and Robert J. Woods. GLYCAM06: a generalizable


Laikov:2007:NFA


Li:2003:HDM


Liivat:2005:DFF


Lipkowitz:1999:RCC


Li:2005:DPT


Liu:2008:ETS

REFERENCES

Liang:2008:PDD


Levashov:2007:QCP


Liu:2006:MCH


Lai:2007:COR


Liegeois:2009:VRO


Lii:2003:AECc


[LD05a] Maxence Launay and Richard Drouskowski. A theoretical study on the structures and energetics of hypothetical

Liao:2005:GAA


Lee:2007:DIC


Luo:2002:APB


Liu:2009:TDD


Lacaze-Dufaure:2001:IMM


REFERENCES


Latek:2007:PSP


Luttmann:2009:AMD


Liu:2002:CRI


Li:2004:CMTa


Leaver-Fay:2007:MSA

REFERENCES


[LFS+07] Carlos Silva López, Olalla Nieto Faza, José A. Souto, Rosana Álvarez, and Angel R. De Lera. Pseudopericyclic design drives

[271]


[Li:2004:CMTb]


[Li:2002:TIE]

Lins:2005:NGF


Lee:2009:BHR


Lee:2006:ABS


Linnolahti:2001:GPB


Li:2007:SRS


Li:2001:ETB

Xiang-Yuan Li. Electron transfer between tryptophan and tyrosine: Theoretical calculation of electron transfer matrix


REFERENCES


Lu:2007:SSH


Li:2008:QSM


Lammers:2008:RFF


Lopes:2009:PEF


Liao:2003:PAD


[LLXS02] Qian-Shu Li, Rui-Hua Lü, Yaoming Xie, and Henry F. Schaefer III. Molecules for materials: Germanium hydride neutrals and anions. Molecular structures, electron affinities, and thermochemistry of GeH$_n$/GeH ($n=0$–4) and Ge$_2$H$_n}$/Ge$_2$H ($n=0$–6). *Journal of Computational Chemistry*, 23(16):1642–1655, December 2002. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Loer:2006:WED


Li:2002:LSL


Le:2001:ISC


Lee:2000:MBI


Liddell:2004:ASS


Luo:2009:AES

Yi Luo, Satoshi Maeda, and Koichi Ohno. Automated exploration of stable isomers of H$^+$($\text{H}_2\text{O}$)$_n$ ($n = 5–7$) via ab initio

**Lopez-Martinez:2009:TSE**


**Larin:2007:QSE**


**Liu:2001:RGC**


**Loeffler:2003:MBE**


**Liu:2008:RIT**


July 30, 2006. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


[Lai:2008:TCH] Chin-Hung Lai and Ming-Der Su. Theoretical characterizations of HAexXH (X = N, P, As, Sb, and Bi) isomers in the sin-

[Lie:2008:DSS]


[Liu:2008:EBO]


[Leininger:2001:SSS]


[Lange:2006:FGA]


[Li:2004:MHA]


[Lee:2004:EHE]

Michael S. Lee, Freddie R. Salsbury Jr., and Mark A. Olson. An efficient hybrid explicit/implicit solvent method for

[Larin:2008:CEF]


[Lubber:2001:CSD]


[Liang:2000:MMM]


[Lu:2002:GTN]


[Li:2007:EPT]

Larin:2008:EFC


Lu:2009:GEA


Leherte:2008:CMR


Li:2004:DDS


Liao:2004:NGR


Liu:2006:RPS


Yongjian Li, Jian Wan, and Xin Xu. Theoretical study of the vertical excited states of benzene, pyrimidine, and pyrazine by the symmetry adapted cluster–configuration interaction
REFERENCES


**Liu:2009:COR**


**Lin:2009:NHD**


**Li:2007:QCS**


**Liu:2007:NCC**


**Liu:2008:SOI**


**Li:2009:NMP**

[LXW+09] Shuyan Li, Lili Xi, Chengqi Wang, Jiazhong Li, Beilei Lei, Huanxiang Liu, and Xiaojun Yao. A novel method for protein-
REFERENCES


Xiao-Jing Liu, Chuan-Lu Yang, Xiang Zhang, Ke-Li Han, and Zi-Chao Tang. Theoretical study on the structure and formation mechanism of $[\text{C}_6\text{H}_5\text{M}_m]^- \ (\text{M} = \text{Ag, Au}; m = 1–3)$. *Journal of Computational Chemistry*, 29(10):1667–1674, July 30, 2008. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


[LZZC09]  Huaiyong Li, Siyuan Zhang, Shihong Zhou, and Xueqiang Cao. Investigation of chemical bond characteristics, thermal expansion coefficients and bulk moduli of $\alpha$-$R_2MoO_6$ and $R_2Mo_2O_7$ ($R =$ rare earths) by using a dielectric chemical bond method. *Journal of Computational Chemistry*, 30(12):
REFERENCES

Mobli:2005:QV

Miura:2009:ITT

Martinez:2009:PPB

Mackerell:2004:EFF

Matamala:2007:SAI

Mak:2008:RCS


REFERENCES

Marechal:2000:TMH


Martin:2009:CMG


Mitin:2003:PSI


Moon:2006:CQC


McDowell:2003:CSL


McDowell:2008:CSS

REFERENCES

Marun:2005:FCP


Marabotti:2007:NCS


Manojkumar:2005:TIM


Mckee:2007:MHE


Mckee:2007:MNF


Mongan:2004:CPM

John Mongan, David A. Case, and J. Andrew McCammon. Constant pH molecular dynamics in generalized Born implicit


REFERENCES

Mackerell:2004:ETB

Moreira:2007:CAS

Mo:2000:IQM

Ma:2006:LBK

Malrieu:2007:EBE

Milet:2006:RNS
Morales:2000:PTS

Melendez:2000:IDI

Masgrau:2003:DRC

Morreale:2003:CDC

Mandado:2007:CGT
REFERENCES


REFERENCES


[mJlZyL+08] Yue meng Ji, Xiao lei Zhao, Jing yao Liu, Ying Wang, and Ze sheng Li. Theoretical dynamic studies on the reactions
of \(\text{CH}_3\text{C(O)}\text{CH}_3-n\text{Cl}_n\) \((n = 0-3)\) with the chlorine atom. *Journal of Computational Chemistry*, 29(5):809–819, April 15, 2008. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Massova:2002:PKM


Makowski:2006:EAE


Mancera:2004:LPD


Moskaleva:2000:UID


Ma:2000:MPI


REFERENCES

2008. CODEN JCCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


[MML02] Buddhadeb Mallik, Artem Masunov, and Themis Lazaridis. Distance and exposure dependent effective dielectric function.
REFERENCES


Marechal:2006:DSR


Makowska:2005:TCH


Mayaan:2007:CFF


Moad:2007:NVD


Mannfors:2001:PEM


REFERENCES

Morita:2002:WPC


Malcolm:2003:ADI


Malcolm:2003:IAL


Murphy:2000:MQM


Marsal:2002:VTV


Maurer:2004:MAA

Marti:2009:HQC


Meagher:2003:DPP


Mutyala:2007:CRB


Mitra:2009:QAP


Mitchell:2000:MSP


Morita:2001:INI

Shoji Morita and Shogo Sakai. IMiCMO: a new integrated ab initio multicenter molecular orbitals method for molecular


McNamara:2006:CSP


McQuaid:2004:DVC


Monticelli:2008:MSM


MacCallum:2003:CWC


Mediavilla:2009:MHP


Michel:2004:PVG

Julien Michel, Richard D. Taylor, and Jonathan W. Essex. The parameterization and validation of generalized Born mod-

**Muegge:2001:ELV**


**Muino:2005:OCR**


**Manninen:2006:SGB**


**Meineke:2005:OOO**


**Medvedev:2006:ATD**


**Momany:2000:CSC**

F. A. Momany and J. L. Willett. Computational studies on carbohydrates: I. Density functional ab initio geometry op-


REFERENCES


[NLL+09] Bing Niu, Lin Lu, Liang Liu, Tian Hong Gu, Kai-Yan Feng, Wen-Cong Lu, and Yu-Dong Cai. HIV-1 protease cleavage site prediction based on amino acid property. *Journal of Compu-
REFERENCES


Takeshi Noro, Masahiro Sekiya, You Osanai, Toshikatsu Koga, and Hisashi Matsuyama. Relativistic correlating basis sets for...


REFERENCES


[OBT09] Nikolaj Otte, Marco Bocola, and Walter Thiel. Force-field parameters for the simulation of tetrahedral intermediates
Omori:2009:LR


[OCB02]


[OCP02]


[OD09]


[OFB08]


[OFIK09]

REFERENCES

Oakley:2005:LMP


Otsuka:2002:TAE


Ono:2002:CFF


Ozkan:2004:CSP


ODonohue:2000:PNT


Ode:2008:FFP


Yuhki Ohtsuka, Kazufumi Ohkawa, and Hiroshi Nakatsuji. Electron transfer in the $\epsilon$-type cytochrome subunit of the photosynthetic reaction center of *Rhodopseudomonas viridis*: ab


Asim Okur, Bentley Strockbine, Viktor Hornak, and Carlos Simmerling. Using PC clusters to evaluate the transferabili-


Okumoto:2003:CSE


Oda:2005:NAF


Oda:2009:ESA


Okamoto:2009:CTC


Polo:2005:JSB


Petrella:2003:IMN

Pacios:2006:CSP


Panczyk:2007:CIG


Polo:2007:NIB


Patil:2008:GCC


Periole:2009:PFE

REFERENCES

Price:2002:MPF


Patel:2004:CFCa


Price:2005:DCB


Page:2006:CMP


Pendas:2007:CFR


Pendas:2009:SRR

Phillips:2005:SMD


Persson:2000:ICS


Perczel:2000:TDD


Ponec:2005:EPC


Ponec:2007:EPC


Pinsky:2008:SOM

REFERENCES

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


[Perczel:2003:TDD] András Perczel, Anna K. Füzéry, and Attila G. Császár. Toward direct determination of conformations of protein building units from multidimensional NMR experiments. V. NMR chemical shielding analysis of N-formyl-serinamide, a model for polar side-chain containing peptides. _Journal of Computa-
REFERENCES


REFERENCES


Praprotnik:2008:NAA


Partay:2008:NMD


Piacenza:2007:CQC


Parsons:2005:PCT


Pribil:2008:SDP

Pinak:2001:MDS

Pinak:2003:OLB

Porwal:2007:PSP

Perez-Jimenez:2007:MMW

Patra:2004:SCF

Petrella:2005:EEF
Robert J. Petrella and Martin Karplus. Electrostatic energies and forces computed without explicit interparticle interactions: a linear time complexity formulation. *Journal of Com-
REFERENCES


[PO03] Christopher S. Page and Massimo Olivucci. Ground and excited state CASPT 2 geometry optimizations of small organic


Pang:2001:ECP


Prabhu:2008:EII


Prall:2001:VGT


Proschak:2008:SPL


Pristovsek:2002:SSS


Park:2005:NSM

Sanghyun Park, Randall J. Radmer, Teri E. Klein, and Vijay S. Pande. A new set of molecular mechanics parameters

Putz:2004:AHP


Putarch-Ruiz:2002:RCS


Putarch-Ruiz:2003:VSC


Putarch-Ruiz:2008:FCI


Porta:2007:CMM


CODEN JCCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Pomelli:2001:SA


Piris:2009:IDO


Pullan:2005:UPB


Pernpointner:2003:PFC


Pykavy:2007:SQC


Pernpointner:2000:PFC

Prall:2001:SEB


Piquemal:2003:ILF


Piquemal:2004:EIL


Ponec:2003:CSA


Pinsky:2003:SAE


REFERENCES


537–540, April 15, 2001. CODEN JCCCHD. ISSN 0192-8651 (print), 1096-987X (electronic). See [ABBC01b, ABBC01b].

Quapp:2004:RPP


Quapp:2007:FTS


Qu:2004:DFI


Qu:2003:DFI


Ramírez-Anguita:2009:FPDa

REFERENCES

Ramirez-Anguita:2009:FPDb

Rao:2000:MSH

Raos:2000:IMF

Rapallo:2006:AUS

Rankin:2001:DFT

Ren:2004:MGL
REFERENCES

2004. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


Rurainski:2009:CLS


Rathinavelan:2007:ETF


Rathinavelan:2008:NSD


Rulisek:2006:RMI


Reveles:2004:GOD


Ruvinsky:2005:NFS


REFERENCES


August 2000. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


[RRCA08] Francisco Rodríguez-Ropero, Jordi Casanovas, and Carlos Alemán. Ab initio calculations on π-stacked thiophene dimer, trimer, and tetramer: Structure, interaction energy, cooperative effects, and intermolecular electronic parameters. *Journal


**REFERENCES**


REFERENCES

Ruvinsky:2007:RBE


Rosta:2009:ARC


Ren:2009:DEE


Rutkowska-Zbik:2007:TDF


So:2007:VEE


Salvador:2006:GEI

REFERENCES


Smith:2002:RQC


Sgrignani:2009:IDS


Simpson:2009:MSA


Strassner:2002:MPF


Santoro:2008:CTD

Schluttig:2008:CMD


Seda:2005:SES


Schaefer:2001:EAV


Sherer:2001:QCC


Shao:2004:DLS


Sousa:2009:CAP

[SCF+09] Sérgio F. Sousa, Emanuela S. Carvalho, Diana M. Ferreira, Isabel S. Tavares, Pedro A. Fernandes, Maria João Ramos, and José A. N. F. Gomes. Comparative analysis of the performance


Seeliger:2009:TGV


Sefcik:2002:DCE


Sun:2007:CSE


Salisburg:2009:RTP


Suarez:2002:MDS

REFERENCES

Schuler:2001:IGF


Stepanenko:2007:GTS


Stepanenko:2008:NTS


Schwobel:2009:MHB


Seno:2006:ATS


Shen:2005:SMF

Sabzyan:2007:EFE


Soler:2004:FTA


Sousa:2007:TSF


Smedarchina:2001:DPC


Steiger:2001:LSC


Schreiber:2007:SBA

[SG07a] Marko Schreiber and Leticia González. Structure and bonding of Ag(I)–DNA base complexes and Ag(I)–adenine–cytosine
REFERENCES


Shaik:2008:CGV

Sandberg:2009:CAH

Shalabi:2002:FAF

Shaw:2005:FSM

Shai07

Schreiber:2005:EEL
Andreas Schreiber, Michael Humbert, Alexander Benz, and Ursula Dietrich. 3D-Epitope-Explorer (3DEX): Localization

Song:2008:MMP


Siegert:2007:GDP


Soares:2005:INA


Shah:2004:PRP


Schwarzl:2005:NCS

Siegbahn:2001:MAM


Simoes:2007:EBW


Shen:2004:HPS


Sun:2009:APE


Sun:2005:UIF


Seo:2008:NSC

REFERENCES


REFERENCES


---


[SLL+04b] Li Sheng, Ze-Sheng Li, Jing-Yao Liu, Jing-Fa Xiao, and Chia-Chung Sun. Theoretical study on the rate constants for the $\text{C}_2\text{H}_5 + \text{HBr} \rightarrow \text{C}_2\text{H}_6 + \text{Br}$ reaction. *Journal of Computational Chemistry*, 25(3):423–428, February 2004. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


References

Sanchez:2000:SEM

Stoll:2002:REC

Song:2009:MIP

Schlund:2008:CAA

Shukla:2000:ISE

Spiegel:2008:PAB
Katrin Spiegel, Alessandra Magistrato, Patrick Maurer, Paolo Ruggerone, Ursula Rothlisberger, Paolo Carloni, Jan Reedijk,


[SPF+07] John E. Stone, James C. Phillips, Peter L. Freddolino, David J. Hardy, Leonardo G. Trabuco, and Klaus Schulten. Accelerating molecular modeling applications with graph-


REFERENCES

Sigfridsson:2002:RPC


Swart:2006:PAM


Seok:2003:MMO


Shi:2008:PSI


Skowronek:2000:WDC


Sateesh:2007:TDS


REFERENCES


REFERENCES


[SURG06] Hugo R. R. Santos, Gregori Ujaque, Maria J. Ramos, and José A. N. F. Gomes. QM/QM study of the coverage effects on the adsorption of amino-cyclopentene at the Si(100) surface. *Journal of Computational Chemistry*, 27(15):1892–1897, November
REFERENCES

30, 2006. CODEN JCCCHD. ISSN 0192-8651 (print), 1096-987X (electronic).


[SWM04] Peter A. Sims, Chung F. Wong, and J. Andrew McCammon. Charge optimization of the interface between protein kinases


Shao:2008:DLS


Shi:2003:ESF


Szabelski:2008:SSH


Schultz:2008:BAD


Suo:2005:PMB


Tafipolsky:2007:IPM

REFERENCES


Thompson:2003:PCM


Tokmachev:2006:EGF


Tchougreeff:2008:CSC


Tye:2006:CBC


Tsipis:2007:GFE


Torras:2008:VAG

REFERENCES


[TGLL07] Ismael Tejero, Àngels González-Lafont, and José M. Lluch. A PM3/d specific reaction parameterization for iron atom in

**Tan tillo:2002:TSD**


**Takahashi:2001:HQM**


**Tielens:2009:ERF**


**Taylor:2003:FFL**


**Takahashi:2003:TSM**

REFERENCES

Togo:2008:FPL


Tsuneda:2003:RSI


Tew:2007:ECM


Tsuchimochi:2008:ASS


Takahashi:2001:TPV


Tappura:2000:NSC

[TLKT00] K. Tappura, M. Lahtela-Kakkonen, and O. Telemann. A new soft-core potential function for molecular dynamics applied to

**Tielens:2000:QCC**


**TMBM02**


**Tuzun:2000:CIC**


**Torii:2002:ICM**

*Hajime Torii. Intensity-carrying modes important for vibrational polarizabilities and hyperpolarizabilities of molecules: Derivation from the algebraic properties of formulas and applications. Journal of Computational Chemistry, 23(10):997–1006, July 30, 2002. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).*

**Totrov:2004:AEG**


REFERENCES

Torrent-Sucarrat:2007:QHK


Torrent-Sucarrat:2008:HKB


Tokura:2008:DLS


Tokmachev:2001:SIS


Tsipis:2002:MAD


Tokmachev:2005:TPS


Tran:2001:CATa


Tran:2001:CATb


Toropov:2009:QME


teVelde:2001:CA


Tautermann:2003:EMA

Christofer S. Tautermann, Andreas F. Voegele, Thomas Loerting, Peter Kaps, and Klaus R. Liedl. Extended method for


REFERENCES


REFERENCES


[Var09] A. J. C. Varandas. Möller–Plesset perturbation energies and distances for HeC₂₀ extrapolated to the complete basis set
REFERENCES


REFERENCES


S. J. A. van Gisbergen, C. Fonseca Guerra, and E. J. Baerends. Towards excitation energies and (hyper)polarizability calculations of large molecules. Application of parallelization and linear scaling techniques to time-dependent density functional

Villar:2005:ALP


Verma:2007:AAN


Vchirawongkwin:2007:QMM

Viwat Vchirawongkwin, Thomas S. Hofer, Bernhard R. Rando

Vchirawongkwin:2007:TSS

Viwat Vchirawongkwin, Thomas S. Hofer, Bernhard R. Rando
dolf, and Bernd M. Rode. Tl(I)-the strongest structure
breaking metal ion in water? A quantum mechanical/

Vemparala:2006:ICI

Satyavani Vemparala, Ivaylo Ivanov, Vojislava Pophristic, Ka


J. H. van Lenthe, H. B. Broer-Braam, and Z. Rashid. Letters to the editor: On the efficiency of VBSCF algorithms,
REFERENCES


VanDerSpoel:2005:GFF


Vreven:2000:AI


Villa:2002:CFE


Vila:2007:AMI


Vetere:2003:CSQ

REFERENCES


REFERENCES

Vijayalakshmi:2008:TSC

Vadali:2004:SFG

Vaiana:2003:MMF

Voltz:2008:CGF

VandeStreek:2002:IEC


REFERENCES


REFERENCES

November 30, 2005. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


REFERENCES

Wang:2001:APP

Wong:2008:TCM

Widjaja:2002:PCS

Wheatley:2008:TDC

Wittayanarakul:2008:APP
Woodcock:2007:IQC


Wu:2006:DDS


Wang:2002:APP


Whitnell:2008:CMV


Wiberg:2004:BSE


Williams:2001:IIFa

REFERENCES


Jia-Yan Wu, Jing-Yao Liu, Ze-Sheng Li, Xu-Ri Huang, and Chia-Chung Sun. Dual-level direct dynamics studies for the reactions of dimethyl ether with hydrogen atom and methyl

[Wang:2007:IDD]


[Wang:2007:TSR]


[Wang:2004:DID]


[Wang:2005:TSR]


[Wang:2005:PCS]


Gui-Chang Wang, Jun Li, Xiu-Fang Xu, Rui-Fang Li, and Junji Nakamura. The relationship between adsorption ener-


REFERENCES


REFERENCES


CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Wei:2008:ATM


Wei:2009:PCT


Watanabe:2006:RGB


Wu:2006:ESM


Wang:2003:PEM


Wiberg:2004:CES

REFERENCES


REFERENCES

2442, November 30, 2007. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


[XFF06] Ju Xie, Dacheng Feng, and Shengyu Feng. Theoretical study on the isomeric structures and the stability of silylenoid (Tsi)Cl_{2}SiLi (Tsi = C(SiMe_{3})_{3}). *Journal of Computational Chemistry*

Xu:2008:USS


Xue:2005:DSM


Xue:2002:TSG


Xie:2002:TSG


Xiao:2008:UGD


Xiao:2006:UPA


Xiao:2009:GCC


Xu:2009:NED


Xie:2008:EEA


Xi:2006:DGQ


[YDWS06] Li-Ming Yang, Yi-Hong Ding, Qiang Wang, and Chia-Chung Sun. Monosilicon-substituted cyanoacetylene: a computational study. *Journal of Computational Chemistry*, 27(5):578–
REFERENCES

Yang:2005:TSE


Yanover:2007:DEE


Yu:2006:MDS


Yang:2005:MAO


Yoshida:2006:NMD


Yoshizawa:2007:CFD

Terutaka Yoshizawa and Masahiko Hada. Calculations of frequency-dependent molecular magnetizabilities with quasi-


REFERENCES

Yim:2008:AMA


Yuzlenko:2009:MMA


Yang:2006:GAP


Yang:2009:SMN


Yu:2009:CSR


Yang:2008:TSR

[YLW+08] Lei Yang, Jing-Yao Liu, Li Wang, Hong-Qing He, Ying Wang, and Ze-Sheng Li. Theoretical study of the reactions CF₃CH₂OCHF₂ + OH/Cl and its product radicals and parent


References


[Yan:2009:EED]


[Yamabe:2003:CSI]


[Yamabe:2004:CSR]


[Yanagisawa:2001:IUD]


[Yuki:2007:IIM]

REFERENCES


[YXZ+04] Weizhong Yan, Ying Xue, Hua Zhu, Jun Zeng, and Daiqian Xie. A theoretical study of solvent effects on tautomerism and electronic absorption spectra of 3-hydroxy-2-mercaptopyrindine...


[ZAT07] Jingjing Zheng, Ahmet Altun, and Walter Thiel. Common system setup for the entire catalytic cycle of cytochrome


Zhan:2005:FPS


Zerara:2008:PCP


Zhu:2005:CMT


Zhou:2008:HAB


Zhang:2001:SMP


Zhu:2006:IPE

[ZGXX06] Hua Zhu, Yong Guo, Ying Xue, and Daqian Xie. Ab initio potential energy surface and predicted microwave spectra for

Zhu:2007:CIS


Zhao:2008:TDD

Zhao:2009:FPI

Zou:2009:HPQ

Zhou:2006:RCP

Zeng:2007:EAH


Zhao:2007:CDQ


Zou:2005:ETS


Zou:2007:TSL


Zhu:2009:NME


Zou:2009:CIC

 Zheng:2009:STC


Zacharias:2003:PSM


Zhang:2004:TSR


Zhang:2004:TSM


Zhang:2005:TSR


Zhang:2006:TMS

[ZLLS06a] Jia-Xu Zhang, Ze-Sheng Li, Jing-Yao Liu, and Chia-Chung Sun. Theoretical mechanistic study on the radical-molecule

**Zhang:2006:TSM**


**Zhang:2007:NID**


**Zyubin:2003:PTD**


**Zoete:2006:IIS**


**Zyubin:2009:QCM**

REFERENCES


REFERENCES


Zhang:2009:EIM


Zhou:2009:CA


Zhou:2009:FF


Zhang:2005:DLD


Zhong:2008:TSP


Zicovich-Wilson:2004:CVF

C. M. Zicovich-Wilson, F. Pascale, C. Roetti, V. R. Saunders, R. Orlando, and R. Dovesi. Calculation of the vibration frequencies of α-quartz: the effect of Hamiltonian and
Zheng:2002:SSE


Zhang:2009:MDS


Zicovich-Wilson:2008:ISI


Zheng:2009:DSC


Zheng:2009:ITS

REFERENCES

Zeng:2004:HBS


Zhu:2008:ISE


Zhu:2009:SPH


Zhao:2004:ACT


Zhu:2003:TSS


Zhang:2008:SIG


REFERENCES


**Zhang:2008:EPW**


**Zhang:2006:ISI**