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Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA
Tel: +1 801 581 5254
FAX: +1 801 581 4148
E-mail: beebe@math.utah.edu, beebe@acm.org, beebe@computer.org (Internet)
WWW URL: http://www.math.utah.edu/~beebe/

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Title word cross-reference

($\Phi$, $\Psi$) [WD04]. ($\varphi$, $\psi$) [TTB01b]. –2 [ZZZ'06]. –4 [ZZZ'06]. 1 [FROD08].
$1/r^p$ [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 $\leq N \leq 372$ [Pul05]. $\$$3 [Lip00]. 3
[BAB'+02, FROD08, GDPCPU07, GdSuM'+07, HP05, mJLzyL'+08, KSN01,
LYZ'+08, MP03b, PF06, SHBD05, SFC04, TJM'+03, WLL07a, WDZS07,
XLL'+02, ZLY07]. 3,10 [JS07b]. 3d [Hol05, LD05a, Wu06, SZT08]. 4
[FHF'+01, LLXS02, QB05, WDX'+02]. 4,7 [ZWS'+02]. 4d [ABYMO08]. 5
[ZXL'+04]. 5d [HZ09]. 6 [Han01, LLXS02]. 7 [LMO09]. 8 [KS05a]. 9 [UM03],
[n] [VKP'+08]. ## [BRV'+07]. +
[FKS'+09, GLRL02, GSPS06, GWL07, HDO'+02, ITS06, KT08, LMO09,
Mck07b, PV07, Sha02, WWT08, ZYW'+09, ZL05, dRLMS00]. +2 [PNG08]. –
[Bac09, Dib05, HTN03, LYZ'+08, Mas01a]. 1
5

3 [AAP00, KAK+09, LEV+09, NYTH09, Rud05c]. 3-butyadiene [Hir08, WR07]. 3-dihydroxy pyridine [YXZ+04]. 3-dimethylallene [ZPL07]. 3-fluorobutanal [NSB08]. 3-hydroxy-2-mercaptopyridine [YXZ+04]. 3-dimethylamino-benzonitrile [ZH08]. 3-dithiacyclohexane [FD03]. 3-dithiane [FD03]. 3-spinor [PV03]. 43C9 [CBS+03]. 45-ns [SO07]. 4d [CWWS07]. 4R [BISB02]. 4R-hydroxyproline [BISB02].

4 [Lu09]. 4-carbonate [vDSSvA04]. 4-dihydropyridine-based [HSMT04]. 4-dimethylamino-benzonitrile [ZH08]. 4-dithiacyclohexane [FD03]. 4-dithiane [FD03]. 4-Spinor [PV03]. 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-carboxybenzisoxazole [UTH+03]. 5'-phosphate [PMM05]. 5'-phosphate-dependent [LDY+08]. 5-phospho- [RGP+07]. 500-MHz [CMD+04]. 53A5 [OVMV04]. 53A6 [CLWL09, OVMV04].


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

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

9-heterofluorenes [CZF07].

= [Bac09, CPJ00, CRC+08, GHLK+02, GPSP06, Han01, HT05, HYA02, HKHN08, HZ09, Hua09a, JJK+00, KBL08, LS08a, LZZC09, LYA+08, Mar03, Mck07a, Mck07b, OS08, RB01, STC+08, WLLS04, WZZ+09, WD08, WWS07, XFF06, ZJM+07, ZY01, ZXY03, ZLO9b].

A*0201 [WCF04]. AA [KB02, KDSV02, POJ01, PB05, XLT07]. AA/L [KOML08]. Ab-initio [Ha08, 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, mJZsLyL07, LW04a, LLL07, TGLL07, WLLS04, XLL+02]. Ac
[GHLK+02]. accelerate [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, UBDPJ04, Bie04b, FKFG08, JS07b, KC01b, MKGA06, MHW04, RK05, SM03, SW06]. Accurate
[ABWT09, BpPRMAI00, EK06, GK09, Grl04, Hdl06, HD06, HMSM06, Ish04, LLZL09, MSH+06a, Tot04, WFHP01, WHP02, WHF08, WX09, ALKH04, Bie04a, BLB09, CGBF05, CF06, GKK07, HdlD05, JKK+00, Rud05a, Rud05b, Rud05c, Vas02, WCC08, ZFW08, vEMK01]. accurately
[IGL07, SBI08]. acetaldehyde [Lu09, YLZ08, Lu09]. Acetalization
[RUPH06]. acetals [MG06]. acetamide [CCK01]. acetate
[GWM08, PGG06]. acetic [MH08a, YT03]. acetonitrile
[ELK+09, GJK00, NL07]. acetylene [DLD+02]. AcF [GHLK+02]. acid [CJK+02, CML05, CSDK09, CK01, DP03, DP04, DLHC06, DHW+07, FZL07, HFHL06, HLC09, IT03, IKYM09, JPF+00, JKM08, JCL05, KLB03, LL07, MT03, MMLC05, MSF+08, MOH08a, Nak07, NH05, NLL+09, Pac06, RR05, RKK03, SKGS00, SYC03, SL04, SBG09b, SRW06, SHK+05, UNHT06, VM02, XSHC06, XLC08, XLT03, YTL03, YXL+09, ZZY07, ZZY08, ZOJ+06, vDSSvA04]. acid-3
[vDSSvA04]. acid-catalyzed [RR05]. acid-nucleotide [MSF+08]. acidity
[ELK+09]. acids [BE06, CADW03, CLA+00, FM00, HWTL03, HP04, IKYM09, KS01a, LD+08, MB00, MM05, NHH05, ONM08, PPYS08, VAn02a, XKKL03, YLL+09, ZLD09]. AcO [GHLK+02]. across
[HZX04, SSM08, SRB06]. act [GM01]. actinide
[AB00, GHLK+02, NSO+07, VAM03]. Activation
[EL06, BGC+09, BZL05, CC09, CFER04, KT08, Lu09, PV07, RRS06, Vya01]. active [AG00, BSDM04, CFR06, CFS+09, FCP+04a, FCP+05, HBM06, HFS+07, HYR06, JHPRSM+05, KSK00, KZO03, LLL03, MDA08, PFM06, RZWS07, SS05, SFR07, TDH06, XLL08]. active-site [SFR07]. activities
[HMMS09, MS04, ZWB09]. activity
[AGMPRG+08, Bou01, CW02, DD08, DA01, DHW+08, DHW+09, FTLV01, GDP08, LC09, MRS09, Sha02, WZY04, Zer08]. acylation [MCK05, MK02]. adaptable [KF08]. Adaptation [HLM05]. adapted
[FCP+04b, HDS06, HD06, LXW07, PTC01]. Adaptive
[BHW00, HBW01, HW03, HLSH05, DK01, GY08, OM04, RNG03,
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]. 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]. affect
[AST06]. affinities [AVS09, DJ04, KS05a, KKMMS04, LLXS02, MRS+07,
SRB06, WSM+08, ZJM+07, ZXL+04, dSGCG00]. affinity
[AB˚A04, FO08, GCD+08, KFB05, KS08, Lee09, LXW+09, MML+06, RTG00,
SOOF05, SWV+05, ZWB09]. affording [OY01]. after [TJM+03]. Ag
[GPSP06, LYZ+08, NA06, SG07a, WCS09]. against [SSS+09]. AGBNP
[GL04a]. AgBr [Sha02]. agent [LHJ+06]. agent-based
[LS05b]. AgN [ZX08]. agonists [GCD+08, SBG+09a]. Agreement
[LCDA03, LCGA03, LCA03]. aldehydes [LLA01d]. Alder [Hir08].

Alchemical [Blo04]. alcohol [FBGD06]. Alcohols
[ALED03, LCDA03, LCGA03, LCA03]. algebra [AT02]. algebraic
[Tor02]. Algorithm
[GGB07a, GGB07b, JHMB+09, JHMB+11, WWT08, ZWY+09]. alkalimetal
[BSG07]. alkaline
[JHMB+09, JHMB+11]. alkaloid [BMRF01]. alkanes
alkyl [BE06, CC07, EB04, LLZL09]. alkyl-cyanobiphenyl [CC07]. alkylation [EL06, VBGL+00]. alkynes [WCO8]. 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 [WMRW+01, ZKZ+07]. allenes [WCHW09]. allocation [SKSH07]. allomeric [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, JBJB00, JJB02, LMMW04, RFSS06, TCT03, VGGMM05]. AM1-BCC [JBJB00, JJB02]. AMBER [Ano06c, WWC+05, JS07b, JM07b, MRC03, OYH05, TdMSD+08, WCC08, WWC+04, WZW+06, WS07]. AMBER*C [CLA+00]. AMBER95 [ONHN00]. ambiguous [BS01]. Amica [GBL+05]. amidase [CBS+03]. amide [CCK01, GSB09, LKA01, SJW09, YSA+03, IINK09]. Amide-[IINK09]. amides [CMLS05, KS06]. amine [OY03, PS03]. amines [CLFA07]. amino [CADW03, CJK09, CLA+00, DLHC06, DHW+07, FDSA00, HFHL06, HLC09, IT03, IYKM09, JPF+00, KS01a, KLB03, LDY+08, LL07, MT03, MM05, MSF+08, NLL+09, RKH03, SURG06, SKGS00, VM02, XHSC06, XLC08, XLT07, XKG+05, YLL+09, YXL+09, ZLD09, ZOJ+06]. amino-cyclopentene [SURG06]. aminoarabinonucleosides [BL08]. Aminopurine [SC01]. aminoborinonucleosides [BL08]. aminosubstituted [TKS+01]. ammonium [HIT5]. ammonolysis [UNM+01]. among [IGNH03, LL07, WS07]. amorphous [CA04, CA07a, CA07b, SHH07]. AMP [FKM+06, FKM+07]. amplitude [KS05b]. Amyloid [BTP09, MS03]. amyloidogenic [CP09]. amyllose [NK01]. anabolic [AGMPRG+08]. analogs [CGSdST06, EKO+01, HG08, KS01a, LWK08, UTM+02, UT+04, hYDN+08, AJNG01, ALB09, AVS09, BM07, BLF02, BL00, BAH+02, BPCD07, CG03, CS01, CCP04, CSRT04, CA07b, DDKV07, DRAS04, JSR+07, ECM+03, FK07a, FC06, FSS00, Gly06, GS07, Gra07, GHBB04, HHWG08, HS00, HLHS05, HP05, IN08, JPF+00, JMD+02, JFG04, KB02, KK08a, KM02, KS03, KN04, KSS00, KMA+07, Kni00, LR+02, LS05a, MGCA07, MS03, MWE02, MHW04, MFP+07, MA05, NK06, NSU+02, OML+00, ON07, PFC03, PGH+04, PP08b, PYEA03, PAS07, PYCD03, PY05, PC07, PLC08, RMK03, RS07b, SH09, SMGE08, SSHT03, SFC04, SCF+09, SvDS01, TYN05, TCR+02, TT01, TD06, TT01a, TT01b, UTH+03, VGB08, VKCK09, WKBV03, YNW05, YK08, ZSE08, Zer08, ZWB09, ZHH09, ZB07, NYK+09, Ruv07, VB09, RS07a, VB07]. analytic [ASWG07, DOSG06, GL04a, IK00, KBT03, LFSB03a, LFSB03b, SJW09].
Analytical [HNWF07, HNWF12, PDC+08, QCK01, QCK02, RLR+04, WL02, JSR+07, HC08, HHS+05]. analyze [AGMPRG+08, Ham07, MCF07]. analyzing [DW08, LD05b]. andradite [ZWTP+08]. anesthetics [TZX01b, TZX01a]. Anglada [Bof01, Qua01]. angle [CIB05, FWH+07, LIO7, OFIK09, YL06]. angles [FPG+06, Ham07, MCF07]. anharmonic [BP07, DB07, GBDP05, LMO09]. anilido [GTC06]. anilido-imine [GTC06]. anion [JT06, CW02, DMN05, EFQD09, GS04, wQZsLyZ02, QZZZ03, VDM06, WLZ+07]. anion- [EFQD09]. anionic [ALC08, HHWG08, PGG06]. anions [CTFC08, KKMMS04, Lee09, LLXS02, Owe05, ZXL04]. anisotropic [BCIB05]. anisotropy [GKTS04]. ANN [HSMT04]. annealing [ADM+06, CS02, CCP04, HPP00, KH01, LCKL05, LJKL08, MCF05, WG02]. annexin [MHJS06]. Announcement [Nor04]. Announcements [Ano05a]. annulation [GLH+08]. anomeric [CPJ00, CPJ01, CKF01, LCDA03, VM07]. ant [CLZ+09, CLZX09, DDKV07]. antara [LFS+07]. antara-antara [LFS+07]. anthracene [CG08, CDPL09, HIA03]. anthracene-9 [CG08]. antibacterial [YCW+09]. antibody [CBS+03, SOOF05, TH02, UTH+03]. antibody-catalyzed [TH02]. anticancer [BZL05, PFR04a, SMM+08]. antifungals [GDPP08]. antiinflammatory [CMBC08]. antilipid [MRS09]. antimicrobials [GDPP08]. antitumor [KC01a, WM01]. apatite [RD06]. Applicability [DC02, PRS04, QTdG+08]. applicable [PB05]. Application [ASDP+06, CIB05, GWS+02, HKMS01, HSMT04, HM08, HMMS09, KSS08, KAK+09, KBK+01, Mat03, MW09, TBSM09, TKN+08, BLN01, COS01, CSJ01, DLWV07, DV02, FOK+04, FKU+05, GLD08, GWM+00, HHBH06, JW06, JGVF05, KTM02, K01a, LL00, LFSB03a, LFSB03b, LI07, LSHR04, LCSZ09, LXL07, LLL03, LMO09, MG00, MS04, PB04, RI07, Rud05a, SG07b, Tot04, VM00, Wli01b, WR07, ZLY07, ZNL07, dGWH01, CMJ08, CVW+05, CMB08, JSR+07, GRO+03, GBDP05, GS04, IN08, IS03, LJZ+07, LSY02, MB00, MCF05, MBC08, MTB09, ON07, PHJ+08, Qua04, QCK01, QCK02, Rud05b, Rud05c, SL09, SDCG02, SFC04, TH02, VVS07, VKCK09, WRP+06, WFR08, vGGB00]. Applications [HLLN06, BWZ08, BBG+04, CGMPT+08, CR09b, Est07, LW06, PMC+08, PTC01, SPF+07, Tor02, ECP+03, GGB07b, HT03, RSN+02, WH03]. applied [ADM+06, BL09, BT00, BS06, DMN03, FII+07, GHK+02, MKGA06, OM04, TLKT00, YAÇ+02, ZZ08, dVB01, BBC+05]. Applying [AGMPRG+08, Woo01, You11, GS02]. appreciation [vRS01]. approach [AB00, AGK03, AVS09, BG03, BEM05, BS03, BG01a, BLF02, BMSTC01, BPCD07, CCWH02, CYM02, CGFB05, CAGR08, CMBC08, CG05, EM03b, GAIVMB01, GAIO6, GJL+08, GRO+03, GSV, GS02, GDPP08, GdSU+07, GdAcV+07, GCD+08, HMMS09, Hn00, HRR05, HT03, HLSH05, IT03, KKG+09, KN04, KHY00, KHF+09, KBT03, LFKL00, LCC09, LMJ02, LYS08, LD05b, LWZ09, MAF+07, MR04, MFR07, Mor02, NYTH09, Oos09, PS09a, SAM06, SPGS08, SGPS09, SL04, SWZS04, VV03, Van02b, WWL+09].
XWC09, XKKL03, YS00, YK08, ZCS04, 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, SZ07, SYC03]. **approximated** [PSF+08]. Approximately [EA06], **approximating** [MR04]. **approximation** [AB09, BRS00, BRS01, CLP+05, CCK01, Der09, EA08, GMA04, GWS+02, ION07, Kri09a, Lai07, LFSB03a, LFSB03b, LN01, MTE04, Nee03, OCB02, RP07d, SHSF05, ZFL+05]. **approximations** [Dya02]. **APS** [CBC+08]. **APX** [ZJM+07]. **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]. APS [CBC+08]. APX [ZJM+07]. **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]. arabinonohydroxamate [RGP+07]. arbitrary [KH06, LMV07]. architecture [TDK07], architectures [TYO+02]. area [GCC+08, GB04, HHS+05, Lab08, LFBSK07, RP07d, VP02, ZCL09]. areas [BHH+09, TRS02]. arene [FK+09, PCMG09, RRZ08]. arene-containing [RRZ08]. arginine [CJPZ08, SMGE08]. arginine-bound [CJPZ08]. argon [BWW+08]. argument [Ish04]. ARIs [PS09a]. arising [CCSJ00]. armed [KLM+09]. ArOCS [ZGXX06]. Aromatic [CPML08b, FV08, HLC09, MM05, MGMM07a, ST01, SMV+09, TDK07, VS08, WFP01, XL07, PCO+07a]. Aromatic-Backbone [CPML08b, Van08, PCO+07b, PCO+07a]. aromatic-type [HLC09]. Aromaticity [BPCD07, FMP08, HJMB+09, HJMB+11, LWW+06, LTF+07, MGMM07b]. Array [FJP07, ABF+03]. arsenic [ALC08, KS05a, ZXL+04]. ARTE [VB07]. ARTE-QSAR [VB07]. artifacts [CCSJ00]. Artificial [PS09a, RBW08, VB01, CLC03, Gol09, NINAT+07, TCSM03]. arylamide [VIP+06]. ascorbate [HBM06]. ASIC [NYTH09]. aspartic [ZZY08]. Aspects [HBH00, MO01, BMRDB01, BRS07, Sie01, TT02]. assemblies [DFG09b]. assembly [DPRR05]. Assessing [IB04, FGR07]. Assessment [BP03, CCWH02, DGI+08, KS08, LWH06, SSS+09, WSM+08, CKMC04, FPMS08, GT03, LLS03, SP05, GGT08, GBB04, TFZRG01]. assignment [BB05, BMRF01, PRJ02]. assignments [PF06]. assisted [BA04b, KT08, WJ+08]. assists [BM07]. associated [SRW06, TT08]. Associative [ABYM08, NL08]. asymmetric [WR07, WFR08]. Asynchronous [GLP08]. atmospheric [GCCVB00, PGNG03]. Atom [BP07a, RM00, BPC01, BR04, BWW+08, CCK01, FM00, GWS+02, GB04, HLLS05, IT03, JS07a, mJLZ+08, LMK01, MT03, MB00, PHH+08, RG08, RS08, SSB+03, SBLK01, SLL+04a, TG07, VK06, VGO+07, WLL07a, WBSR03, WS07, WLL+03, YLWL09]. atom-bond [VK06]. atom-centered [SBB+03]. Atomic [DVP+02, FM00, AS00, BAC07, BSC+01, BCN07, BSP06b, BK00, BLT03, BAA07, CN03, FS04, GC02, Ish03, JBB00, JJB02, KRM+02, Kau07, KS01a, KCO1b, Lab08, LMV07, LST08, LTV08, Nl09,
atomic-centered [TBSM09].
atomistic [CA04, IDMC09, KK01bb, RPMP03, SPGS08, ZALMG03].

Atoms
[VM07, YK08, ALTB06, AD00, ASS+02, BHTCG07, BKS02, BS03, CMJ08, CDS09, EdlVR+03, FS04, HSF08, mJiZsLyL07, KGN07, KS02b, LDC+07, Mat03, NSO+07, RP07b, RRP+01, RLR+04, RLER04b, SO09, SNM+06, SFC04, Wi01b, WDX+02, XLL+02, PF05].

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
[JˇCHS07, 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].

automaton
[XWC09].

auxiliary
[GKH05, JSHG07].

available
[SCF+09].

averages
[Rap06].

averaging
[BSC+01].

avian
[DLRZ09].

avoidance
[WCFH02].

axial
[BMRF01, CN05].

axis
[OMNH08].

azaglycine
[LKJ+04].

azole
[SMM+08].

azole-bridged
[SMM+08].

azurin
[PMGL03].

B
[OS08, Sta00, WZZ+09, WD08, ZZZ+06, ALKH04, BAL+01, FH01, GL04b, JS07a, KVS+06, LMG06, MZ06, ZWB09].

B-DNA
[M01, Pin03].

B-domain
[JS07a].

B-spline
[ALKH04].

B-splines
[GL04b].

B3LYP
[CLP+05, FSFK05, HWG01, NL08, TCT03, WC04, WX09].

B3LYP/6
[FSFK05, NL08].

B3LYP/6-31G*
[NL08].

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

Ba
[WD08, XB08].

Bacitracin
[Dra00].

back
[BB05].

Backbone
[CPLM08b, GKK07, Van08, Adc04, An06c, AHG09, CLW09, HSW01, KL01, LHA01, MBL08a, PC0+07b, SP05, WZ+06, YL06, PC0+07a].

backward
[KM07].

bacterial
[An06b, CPM03, GSS04].

bacteriochlorophylls
[LKT04].

bacteriochlorophyllin
[IN01].

bacteriorhodopsin
[RG02].

Bacteroides
[SDM02].

Bader
[GHBB04, SKSH07].

Baker
[WB05].

balanced
[An06c, WZW+06].

balanced
[PB05].

Balancing
[CF06].

band
[AJ03, JCA+02, ZZ09].

Baoshan
[JW12].

bare
[KT08].

barrier
[CRGN07, KSTC01, LSG06, MG06].

barriers
[DBM03, EL06, HFL06, PBF09].

base
[CCK01, DP04, FZL07, HWL03, KMK04, MML05, MFS+08, MHS05, NL08, OY01, PG04, PSS+04, PSB05, SKG00, SG07a, ŠBL05, SC01, SJC03].

base-catalyzed
[OY01].

base-pairing
[DP04].

based
[Adc04, ALTB06, ALB09, AB09, BDPRA100, BMR01, BDW00, BMTSC01, CGM+08, CRK08, CLZ+09, CLZ09, CTK08, CHA+07, CPUGD09, CMB08, CRGN07, CA04, CSB+03, DLW06, DML05, DHW+00, DB102].
DDVD09, DHW+07, DHW+09, DWC+03, FCK+08, FCP+04a, FCP+05, FM00, FZL+06, FRLN09, GZL02, GRCD01, Gon07, GDPCPU07, GDPP08, Gra07, GAS04, HSMT04, HS07b, HLM05, HZ06a, HZ06b, HMOG07, IIK09, IR03, JD09, JKI08, JGF05, KLS02, KBA+04, KK08c, KKB+01, Kob03, KIM+09, KZW+05, KVS+06, LFKL00, LHJ+06, Leh06, LXZ06, LJZ+07, LH05, LM09, ML06, MSF+08, MSH+06a, MBH+02, NLL+09, NMAT01, OVMV04, PS09a, PFR04b, PA05, PAS07, PRJ02, PF06, PRDS08, Pul05, QHL09, Rao00b, RSE09, RLD09, RSN+02, RKA+09, RUPH06, RRS09, RSS09, Ruv07, SAM06, SKSH07, SGL09, SPL+02, SBB02, SE08].

based [SZW+05, TTBM09, Tot04, VSK+04, VB09, VGDSU08, WL09a, WL00, WS07, Ws07, XYN06, XL02, YWZH03, YNW05, YDN08, 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, JJK+00, Wib04, ABF+03, ALK04, Bac07, BY06, BR04, BT00, BS0B05, BRV+07, CMJ08, CRS05, Cul04, CGSdST06, DMZT08, EA08, EdiVR+03, EL09, FZL07, GKH05, HdmD05, HdsO6, HD06, IO08, JSHG07, KK08a, LF05, Lai07, LMV07, LST08, LT08, MV06, Mas04, MLL+08b, MC06, MY08b, MY08a, NSO+07, OBBS05, PSC+01, Pen06, PFJ+03, PS05, RRE01, RLRE07, SSB03, SNM06, TSSSG08, VKP+08, VB03, Var09, VKCK09, WMGK07, WTKM06, Wt08, ZWPR+04].

Basis-set [AHK02, MV06, Pen06, VKCK09].

BCC [JB06, JBJB00, JBJB02].

be [HdM05, HdsO6, HD06, IGL07, STSF02, WCF04, BP01, LWW+06].

beam [BAL+01].

bearing [NL08].

Becke [AAP00].

Becke-3 [AAP00].

Becke3 [PDS01].

Becke3-LYP [PDS01].

beH [PRSMV08].

behave [PB02].

behavior [Ama02b, Bac05, BISB02, LB05, OO04, RP07c, SH08].

behaviors [LML+00].

being [OCB02].

benchmark [Ano01b, BS05, DGD+05].

Benchmarking [Hol05, SZT08, WS07].

Bennett [KBB09].

Benzdiynes [ASY01].

benzene [BE09, BRLS08, BRLS12, HT05, HRG07, IINK09, LWX07, Sch00, SG07b, ZTP+08].

benzenes [PB05, WR+06].

benzo [GLRL02].

benzocryptand [WWT08].

benzodiazipine [SPGS08].

benzodioxoles [MRS09].

benzoic [BE06].

benzonitrile [ZH08].

benzylideneaniline [BY06].

benzylicpenicillin [DS03].

Beowulf [BMRDB01].

Bergman [PWFS01].

Besal`u [Bo01, Qu01].

Bessel [DS08].

Beta [LHI09, BTP09].

Beta-hairpin [LHI09].

between [AD00, AZM03, BS03, CFR06, DRA05, EFQD09, FG03, FL07, FO08, FKM+06, FKM+07, GWM08, HPP00, HRBK03, HFHL06, HN20, Hir08, IINK09, JPC08, KWK+01, KWK+02, LDC+07, Li01, LL01, LFZS04, LLL03, LS05b, MST+08, MBH+02, OY01, PSF+08, PMPGP05, PS03, RLRE01, SM08a, SBLK01, Sim07, SWM04, SKK+07, SP05, TYN05, TK08, TDH06, UTM+02, UTT+04, WLX+05, Y03, YQ09, Ysq02, ZZTS09].

beyond [CLP+05, CCK01, Ha08, PP08b].

BH [QZL+04, SAS05].

Bi [LS08a, WL09b, HZ09].

bi-transition [WL09b].

bias [OM04, SY09].

Biased [MLG04, KV00].

bicyclic [EBDPM00].

bicyclo [BE07, BCP01].

bifurcation.
bilayer [CEP07, HNL08, MCR08]. bilayers [JM07b, RG08].

bimetallic [WCS09]. bimolecular [ML00]. binary [Kle02, Kle03, LCSZ09].

Binding

[ABÅ04, AGO+02, BCP03, RGP+07, ABYM08, AM06b, APG05, AVS09, BWE05, BSP06a, DLRZ09, Dra00, ECM+03, FKU+05, GCD+08, GS04, HT05, HNW07, HNW12, IO08, JMD+02, JZD+09, KFB05, KS08, LXW+09, MK02, MHJS06, MLL+08b, MRS+07, NyHN06, NHN06, OYH09, OFIK09, PMGL03, RSG03, RGG05, Ru07, SOOF05, STSF02, SVW+05, TGGP00, VGGMM05, WM04, WHF08, Won00, XL02, ZGFL01, 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, GdAcV+07, HMMS09, LDTS07, Mac04, TH02, WCK00, YPNE09, vdVGDJ00].

biologically [CSU05, LLL03, RZWS07]. biomarkers [VGDSU08]. biomembrane [WEE01]. biomimetic [FO08].

biomolecular [BHW00, BBM+09, CCD+05, CHB+05, CvG08, FWH+07, JTR05, KAK+09, KYT+08, LS04, OVMV04, WB04a, WB05, WL09a, ZFW08].

biomolecule [ABWT09]. biomolecules [ECM+03, Est07, FEVM01, HMD06, KHY00, MMLC05, QSS01, YNZ+08, YJF06].

bionanosystem [MO09].

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

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

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

bisdipine [ACM+06]. bits [PM02]. black [MBP09]. Blind [GZM09]. block [ATM+07, ASS+02]. blocked [RRS09]. blockers [HSMT04]. blocks [SSB+03]. blood [CRGN07, HMSM06].

Blue [CPDZH08, HRG07, CR02, McD08, SRK+00]. blue-shifted [McD08].

Blue-shifting [HRG07]. BLYP [TCT03]. board [ATMK03, KAK+09]. boat [RP09]. bodies [FS98, FSO0a]. body [CCK01, FII+07, FBGD06, Ike04, Loe03, SM03, TKH07, LR03b]. Bofill [Qua01].

Boltzmann [WB04a, WB05, ABWT09, BHH00, BBP09, BH03, BF04, BF07, GPN01, GCD+08, GGT08, H605, HB00, HBW01, KWHH07, LDG02, NYTH09, PZ08, SAT04, VZM+08, WB04b].

Bond

[CGMPT+08, CRC+08, JG03, MGCA07, May07, SH08, WM12, Bac09, BL06, CML05, CPFL02, CPDZH08, CJW+09, Cul08, DR09, DGD+05, DMZT08, FC01, F008, GYM07, Gr07, GS07, HRG07, HS07a, Hr08, JPCA08, JP09, Kle03, KBL00, LC07, LZC09, LS08c, LS05b, MG00, OO04, Pac06, PSC+01, PYS05, PV07, Ra000a, RM07, RCJ02a, RD00, SEKS09, Sha07, Sim07, SPT+03, SWZ04, SMZW05, SSM09, ST01, SSW+07, TJM+03, Tru07, VK06, VBGL+00, WHRG08, WJ00, XWX08, vLBBR12].

Bond-based [CGMPT+08]. bond-order [LS08]. bonded

[CPDZH08, Gou07, HT03, IO08, LB05, LDL+09, LZF+09, McD08, MH08a, NBTN04a, NBTN04b, NL08, PHFC04, ZH08, vEMK01, vE01]. bonding

[AM07, AG00, Bac04, Bac05, Bac07, BHTCG07, BM07, BSG07, CWW07,
CQ04, CCK01, EFQD09, FLK⁺07, FK07b, Jac09, Kau07, KJP⁺07, KBL08, Kle02, Kle03, KGD06, LW07, LWK08, LDL⁺09, PG01, PYCD03, PLC08, RPNJ07, RP04, RS07a, RS07b, SM08a, SG07a, SCP08, Wil01a, WD08, WWS07, XZ04, X09, Yos02, ZX04, ZW09, ZB07. bonds [Bac05, BUMCMRL00, BRS07, CRC⁺08, DR07, HA04, Mit01, NHH05, O008, PG06, PC05, PC07, SO09, SGD06, SJW09, YT04]. Book [Bic09, Lip00, Sta00, Woo01]. bonds [Bac05, BUMCMRL00, BRS07, CRC⁺08, DR07, HA04, Mit01, NHH05, O008, PG06, PC05, PC07, SO09, SGD06, SJW09, YT04]. borane [Bac05, BUMCMRL00, BRS07, CRC⁺08, DR07, HA04, Mit01, NHH05, O008, PG06, PC05, PC07, SO09, SGD06, SJW09, YT04]. borate [HT05]. Born [LFSB03a, BC06, CF06, DLG00, FOL⁺04, FC06, GZL02, ILB03, Lab08, LFSB03b, MTE04, MCM04, OCB02, Tot04, XL02, YJF06, ZGFL01, ZWZ09]. Born/volume [Lab08]. borohydride [QZL⁺04]. Born [LFSB03a, BC06, CF06, DLG00, FOL⁺04, FC06, GZL02, ILB03, Lab08, LFSB03b, MTE04, MCM04, OCB02, Tot04, XL02, YJF06, ZGFL01, ZWZ09]. both [HdMdS05, HdS06, HD06]. bound [ˇCJPZS08, WC09]. Boundary [BH03, ABWT09, Ara04, BVW04, BF04, BF07, HH04, KWHH07, QSS01, TK08, WM06]. boundary/character [ATBLS04, Ber03, CPDZH08, CCB04, CS01, CRSB03, CTFC08, DGD⁺05, DRAS04, El07, FHF⁺01, GYCW04, GZ07, GB02, HBM06, HYA02, HK07, HA04, IN08, LDMR01, LMK01, Mit01, O004, PRSM03, PV07, RD00, RFSS06, SLL⁺04b, STC⁺08, TYN05, WL05, WL09b, XDS06a, XWC08, ZZL04, ZW09, ZLD09, ZZvRSC08, dRLMS00]. C-PCM [CRSB03]. C12A [BRDC02]. C12A-p8 [BRDC02]. C96 [ONHN00]. Ca [WZZ⁺09, WD08, XWC09, HL09, PNG08]. cation [RUPH06]. CaCO3 [SCP08]. cage [CS01, KFD06, WL05, WL09b]. cages [CJS⁺03, Wan09]. calcium [HSMT04, HL09, LGB⁺09, MIJH06]. calcium-induced
calculates [BE07, GG09, Gra07, LMV07, RSSKB03, RM00, Wib04, WM04, ZXY08, Kle03].

Calculating [Chu07, CG05, DRMD03, DF04, LN01, MC06, PDC+08, PMM05, RSE07, SYC03, WCK00].

Calibration [OKH+02, LLZL09].

calanog [RRZ08]. camphor [AST06].

candes [KBN01]. carbohydrates [ACLD03, HR08, KDSV02, LR03a, LCDA03, LCGA03, LH05, MW00, Sto05, Kyt+08].

carbon [KK08c, LMGR05, BSB05, BG07, CZ05, CDPL09, DWS+09, GKK07, HT05, Kt08, KLS02, KMK01, MMRH07, PAS07, wQzLyZ02, SRS07, Wan09, WSC09, XLZ08, YTH01, YLC08, ZSE08, ZXY09, ZM03, vGGB00, vdVGDJ00].

carbonate [ZWY+09]. carbon-centered [WSC09]. carbon-rich [CZ05]. carbonate [LGB+09].

carbonate [BACJCT01, CSD04, IS07, Kar01, Kne05, KBLP09, OV03, RSIN+02, SFRS01, WW03, YS00].

calculated [BE06, BE07, GG09, Gra07, LMV07, RSSKB03, RM00, Wib04, WM04, ZXY08, Kle03].

calculates [ATMK03].

Calculating [Chu07, CG05, DRMD03, DF04, LN01, MC06, PDC+08, PMM05, RSE07, SYC03, WCK00].

Calculating [Chu07, CG05, DRMD03, DF04, LN01, MC06, PDC+08, PMM05, RSE07, SYC03, WCK00].

Calculating [Chu07, CG05, DRMD03, DF04, LN01, MC06, PDC+08, PMM05, RSE07, SYC03, WCK00].
[vDSSvA04]. **Carbonyl**
[RD00, DLR+08, LL00, LL01a, LL01b, LL01c, LL01d, LL03].
**carbonyls** [BRV+07, LMGR05, PLC08]. **carbobutatin** [WM01]. **carboranes**
[JRJ01, OSA06]. **carboxybenzisoxazole** [UTH+03]. **carboxylates**
[CJPZS98]. **CarC** [BBS06]. **carcogenic** [EL06]. **carcogenicity** [VS08].
**Carlo** [AGSFAL05, AGSAF+05, BR03, BHG03, Der00, FCK+08, FKFG08,
GH07, HMD06, IM06, IYK09, KLS02, KM07, KK05, LML+00, LZA02,
LWG03, MH09, NA06, NCO+05, OM04, SKGS00, SCS07, SB08,
SM08b, SWR06, TS05, XKG+05, ZCS04]. **Carlo-with-Minimization**
[NCO+05]. **carma** [Gly06]. **carrying** [Tor02]. **Cartesian** [LPK07, PHR+05].
**CAS** [PRSM03, BM07, JHRPSM+05, PRSM02]. **CAS-SCF**
[JHP2SM+05]. **CAS-SDCI** [BMB07, PRSM02]. **case** [AB00, AS00,
BUMCMR00, BW+08, BS06, CFS+08, CJPZS05, MV06, MDD04, PDD06,
PGG06, PC00, PO03, JUP06, SB08, SN06, V02a, WRRV03]. **cases**
[BDF+09]. **CASPT** [PO03]. **CASPT2** [KRLD09]. **CASSCF**
[BC04, BC07, DOSG06, WLZ+07, dSVA+09]. **CASSCF/CASPT2**
[WLZ+07]. **Catalysis**
[UTH+03, DSW+09, QZZZ03, TH02, VBGL+00, ZDS+05]. **catalyst**
[VBGL+00]. **catalysts** [YXC+07]. **catalytic**
[CGB+09, KSK00, LS08b, MS04, NTH00, RWBH09, SPT+03, WC08, ZAT07].
**catalyzed** [AST06, BTP09, GVATG03, GLH+08, HSWW00, MCK05, OY01,
PHKG07, RR05, SIE01, TH02, TQLL07, WCC08, WCH09, ZWS+09].
**catastrophe** [PA05]. **cathepsin** [ZWB09]. **cation** [DSB+02, Don08, LB08,
OO04, PV07, QZL+04, SLRC01, VLP00, WLZ+07, WSM+08, WU00, ZL05].
**cation-water** [DSB+02]. **Cationic** [JRJ01, TBG00]. **cations**
[ALC08, GSB09, GS04, GWW07, HIA03, HO05, NSB08, RRS06, SZT08,
WWT08, ZWY+09]. **caused** [LPK07, TT08]. **cavities**
[BCIB05, BHH+09, IME02]. **cavity** [RRZA08, ZFL+05]. **C —** [CJW+09].
**CBR** [FHF+01]. **cc** [Wit04, GYMN07]. **CCH** [KZK+07, KZK+07].
**CCI** [FHF+01, WDZS07]. **cclib** [OLT08]. **CCN** [JDWS06]. **CCSD**
[BBT+09, Lu09, FFP+03, PV03]. **Cf** [GPS06, XBO8, BMR01, BBT+09].
**CD38** [UNHY06]. **CDOCKER** [WRBV03]. **Ce** [SNM+06]. **Ceccarelli**
[An060]. **cell** [Gin07, KVS+06, KS05c, LEV+09]. **cell-based** [Gin07]. **cells**
[CCJ09]. **cellular** [XWC09]. **CeN** [VP08]. **centauric** [PA05]. **center**
[BR07, GGA00, IN01, LAD07, MGGM07a, MGGM07b, NR04, OON01,
SGPS09, TBG00]. **centered** [CCK01, SSB+03, TBSM09, WSC09]. **centers**
[GYMN07, JKL08]. **central** [CMMPT+08, CM09]. **CeO** [CCJ09]. **ceramic**
[HZ040]. **cesium** [HD06]. **CF** [mJZL07, LDC+07, gThDiL+01, UT+02,
UTT+04, WLL+07b, YLW+08, YLW09]. **CFCI** [mJZL07]. **CFF91**
[TTB01a]. **CFMC** [NCO+05]. **CH**
[CPJ00, GBPD05, HTN03, IN08, mJZL08, LW04a, LDT+02b, MGLL03,
MUI05, RD00, SL+04a, TMJ+03, WLL07a, WLL+07b, WDX+02, YLW+08,
ZZ04, ZZW+07, ZZL+08, ZZL+09, HKHN08, FHF+01, GD06, HLLS05,
mJZL07, mJZL08, KZY09, KJH08, LW04a, LWY+09, MM05, Mas01b,
OO04, OO08, SEKS09, SLL⁺04a, SSS⁺09, TJM⁺03, UTM⁺02, UTT⁺04, WLL07a, WDZS07, XLL⁺02, YLW⁺08, ZLLS06b, ZKZ⁺07, dOMSL01. CH/ [MM05, OO08, SSS⁺09]. chain [BHG03, DLW06, Der09, Din00, ENM⁺04, GT03, HFHL06, JPF⁺00, KG02, Kró03, LLA01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chains [Cri04, CA07b, DLHC06, MMLC05, MSR04, VM02, XLT07, ZM06]. chair [BHG03, DLW06, Der09, Din00, ENM⁺04, GT03, HFHL06, JPF⁺00, KG02, Kró03, LLA01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chairs [Cri04, CA07b, DLHC06, MMLC05, MSR04, VM02, XLT07, ZM06]. Chalcogena [HKHN08]. chalcogenides [JT06]. challenge [BHG03, DLW06, Der09, Din00, ENM⁺04, GT03, HFHL06, JPF⁺00, KG02, Kró03, LLA01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. Challenges [BHG03, DLW06, Der09, Din00, ENM⁺04, GT03, HFHL06, JPF⁺00, KG02, Kró03, LLA01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chair [BFK07, OFIK09]. changes [HH04, JO02, Kar06]. chair [BFK07, OFIK09]. changes [HH04, JO02, Kar06]. chameleonic [PA05]. Change [BFK07, OFIK09]. changes [HH04, JO02, Kar06]. channel [CZK⁺09, FCP⁺04a, FCP⁺05, HSMT04, MCR08, RAGLL09b]. channels [CZK⁺09, FCP⁺04a, FCP⁺05, HSMT04, MCR08, RAGLL09b]. challenge [BFK07, OFIK09]. changes [HH04, JO02, Kar06]. channel [CZK⁺09, FCP⁺04a, FCP⁺05, HSMT04, MCR08, RAGLL09b]. channels [CZK⁺09, FCP⁺04a, FCP⁺05, HSMT04, MCR08, RAGLL09b]. characteristic [YGZZ05]. characteristics [LS08a]. characteristic [Wou00]. characterizing [PHJ⁺08]. Charge [CM09, HT05, JKL08, MZ05, SWM04, ZY01, BB05, BSP06b, Chì03, DWC⁺03, ECM⁺03, FHRR07, GY08, GDV03, GGLR00, GY06, GBHB04, HMOG07, IC08, Jac09, JVK09, KS01a, LFZS04, LLS03, OR05, PB04, PMB04, PP08b, PMPGP05, RLR05, RSN⁺02, SL09, San01, SKSH07, SHSF05, SRB02, SvDS01, TCT03, WSM⁺09, WM04, XL02, XLT07, YK08, ZBS03, ZH08, SDCG02]. charge-based [HMOG07]. charge-density [ECM⁺03, XL02]. charge-scaling [GY06]. charge-transfer [GGLR00, LLS03, ZH08]. charged [PPYS08]. charges [BSC⁺01, BCns07, CR09a, CGBF05, DVP⁺02, GBHB04, HS01, JBB00, JBB02, KGl07, KCo01b, LMV07, PG06, RO09, TBS09, TGGP⁺00, UBD04, WMS06, XLT07, YOB⁺08, dSGCG00]. CHARM [BBM⁺09, HNL08, HMD06, JKI08, LLL03, MM05, MMY07, PB04, PMB04, WHG⁺07, WRB03]. CHARMm-based [WRB03]. CHARMm-GUI [JKI08]. CHBr [ZWL⁺05]. CHCl [LDT⁺02a, ZLLS04b, ZLLS06a]. CHELOC [YLW⁺09]. Chebyshev [II02]. chelation [TFZRG01]. Chem [Bof01, HNWF12, Kne05, KWK⁺00, Qua01, Van08, WHG⁺07]. Chemical [BHTCG07, BBC⁺05, GCn03, HLS07, Jac09, MGMM07a, PB07, PYC03, PYS05, WPS02, AM07, AGMPURG⁺08, ATH⁺03, CZFH07, CDD⁺02, CWWS07, DF06, DBS07, DA01, DPM09, DSN03, DMN05, Dra00, DHH⁺07, Fau01, FVB08, FR06, FLK⁺07, FK07b, FHF⁺01, FOO4, GR07, GGB07a, GGB07b, GGB07, GS04, HWFN01, HHP04, JHZ09, KFNH08, Kau07, KBL08, KLo3, KIN⁺09, KC01b, KGD06, LWK08, LZZC09, LHP01, LDT07, LKA01, Mat03, MA05, MC06, NRKH02, OYH05, OKH⁺02, PXP01, PAS08, PFC03, PG04, PHKG07, PC05, PC07, PRS04, PV07, RNB03, RM07, Rud05b, Rud05c, RSS09, RON02, SAM06, SM08a, Sch03, Sch00, Sha07, SC01, SS05, SSW07, SFRS01, SCP08, TLOG00, Tru07, TT02, UNM⁺01, VBS09, VBGL⁺00, VKCK09, WS05a, WFP01, WHP02, WWS07, WZXY07, XYN⁺06, ZB07, ZMH⁺09, HP05]. chemically [AVS09, Bud07, SB01, PP08b].
chemicals [CMGDAC +07]. chemisorption [KKJH08]. Chemist [SH08, Bic09, Gan09]. Chemistries [Duk01, EA08]. Chemistry [Ano05b, Ano06a, Ano06b, Ano06c, GBL +05, vRS98, WB04a, WWC +05, Woo01, You11, tVBB +01, APG05, BW +09, BT00, BMRDB01, BS06, BSJ01, CMGL +04, CFS +08, CPUGD09, CMGDAC +07, CMCB08, CMA +08, DBM03, FJP07, FKRE08, GDPCPU07, GDPP08, GdSuM +07, GdAcV +07, KSB +02, KBA +04, KJVV08, KYL03, KC01a, LX07, MGCA07, MR09, MBP09, MMRVH07, MPF00, Nye07, OTL08, SH07, Sha07, SBB02, SGD06, TKH07, Vis02, Ano01c, Ano04b, LB99, Lip00, Sta00]. chemistry-based [SBB02]. chemists [Pra01]. Chemometric [HPL03, MRS09]. chemometrics [BLF02]. chemotaxis [FC06]. CheY [FC06]. CHF [UTT +04]. CHFOCHF [YLWL09]. Chichester [Lip00]. chief [Lip00]. CHIMERA [NSU +02, PGH +04]. chip [H¨of05]. Chiral [ZPL07, CGMPT +08, Sza08, ZOJ +06]. chirality [CGMPT +08, PDC +08]. chiral [ST04]. chlorinated [DA01, WDZS07]. chlorine [mJlZsLyL07, mJlZyL +08, WLL07a, XLL +02]. chloro [JKM08]. chloroform [CCK01]. chloroform/water [CCK01]. chromophore [DHM +03, HFS +07, KHF +09, XZ05]. Chun [Ano06c]. CI [Ano01b, DHM +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 [FKS +09, CRC +08, DMN05, GZ07, Han01, HYA02, HTN03, HZ09, Hua09a, mJlZyL +08, KBL08, LF02, Mar03, RB01, STC +08, WLLS04, WDZS07, XFF06, ZY01, ZL09b, BS03, HLLS05, mJlZsLyL07, RFS06, SLL +04a, WLLS05, YLWL09, ZWL +05]. class [CKR08, EBD +01, LL07, VIP +06, YNW05, aYDN +08, Car02, PCS04]. classes [CLF +09, KH06, QLHL09, XSHC06, XLC08, XWC09]. Classic [SRE08]. Classical [ATBS04, COL +06, DK01, LLM09, MA05, Nil09, RP07a, ST02, Zho06]. classification [GDPCPU07, dGWH01]. 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]. closo [JRJ01]. closure [CSJ04, DLSVY00, Mak08]. Cluster [AHGK09, CRJ04, BR04, BP01, BG01a, BWI +02, IN08, JHMB +09, KKHJ08, KSTC01, LMJ02, LWX07, LYS08, Mck07a, MS01, Mor02, NK06, PSF +08, SSB07, VDM06, WK0501, Whe08, WJX +08]. cluster-continuum [WJX +08]. cluster/adsorbate [BWI +02]. clustered [FPN +05]. clustering [CCWH02, FZK09, L05a, LOL +08, RLA01, ZS04]. clusters [BP00, BACJCT01, CGG06, CAG07, DBS +02, GBBH09, HXD08, HYR06, JHMB +09, JHMB +11, JG03, KGL07, KDG +09, KZW +05, LML +00, LWLS07, LSJ05, Mck07a, Mck07b, NB04, OS08, PBZ00, Pul05, QB05, SCC04, SYC08, SW06, WLL01, WZZ +09, WCS09, XZ04, YCS07, ZLJS03, ZXL +04, ZWC +09, ZXY03, ZGXX06, Z09, ZB07, Est07]. CM1
Complex [DFGB09, AS06, Bac09, BRS00, BRS01, GC04, HDF+07, HDO+02, HMK02, IV04, IvSV06, Ish04, JLHF03, Kle02, KVS+06, LB05, LDL+09, MM03, MCF05, MY08b, MY08a, NHN06, Pac06, ZWB09].

complexation [AGI+07, HT05, LMMW04, SRK00, SLRC01].

complexed [Pin03, SDM02, WCF04].

Complexes [APG05, AB00, Ano06a, ACM+06, BTP09, BR04, BL06, BM00, BZL05, CZ05, CG03, CBC+08, CSB08, CBH+03, DPT03, DF04, FRS05, FO08, FRLN09, FKŠ+09, GTC06, GL04b, GM01, GPSP06, GPK05, Gri04, GZM09, GRL07, HLLN06, HRC07, IN08, IO8, IGL07, JMD+02, JD09, JCHS07, KT08, KRM+02, KJP+07, LL00, LHJ+06, LPP06, LH02, LMG06, LLS03, LMMW04, LWZ09, LZF+09, LS05b, Mas04, McD08, MJHS06, MSBS01, MLL+08b, NyHN06, NR04, NMAT01, PGG06, QTDG+08, RPN07, RMP01, RRF+03, SG07a, SCF+09, SBH02, ST06, SVV+08, TGGP+00, UM03, VS02, VMA03, VL00, WB07, WWT08, Won09, Zy01, ZBS03, ZWY+09, ZTS09, dVB01].

complexes* [GK09].

complexity [BT00, PK05, XSHC06].

Component [KBA+04, CCT+03, GPSP06, JMD+02, PVdJB00, PV03, SH02, SM08b, Van02b, WG02].

Component-based [KBA+04].

Components [KJVW08, Car02, LL07, TGGP+00].

composition [HM06, KWHH07, LL07, PAS08, XSHC06, XLC08].

Compound [CN05, BR07, HBM06, RD00, XZ05].

compounds [ACLD03, BB08, BLO+02, CYM02, DA01, EDAJ04, EBD+01, FJ08, FROD08, FO04, Go09, Gor01, JLHF03, KFD06, LLA01a, LLA01b, LLA01c, LLA03, LD05a, IWK08, LTF+07, LW06, LCPA03, LCA03, LJJ+07, LL09, MD04, NBTN04a, NBTN04b, PZWG+04, PYCD03, POJ01, RUPH06, SJJ+04, ST01, TTBM09, YCW+09, YSA+03].

Comprehensive [LF02, ZL09b, ZB07, DLR+08, JF+00, SBL05].

compression [BG07, MBWP03].

comprising [Rud05b, Rud05c].

Comput [Bo01, Qua01, Van08].

Computation [BL+06, Car02, CD+02, FZL07, GS09, LFEdL06, TNS00, ATMK03, Gon07, NIK02, PAS08, RK05, WZXY07, ZCZ03, vW06].

Computationally [Ano01c, Ano04b, Ano05b, Ano06a, Ano06b, Ano06c, BLMS08, CZ05, CPUD09, CMG09, CMDB08, CG05, CA07b, GBL+05, GP007, GdSuM+07, HMK02, LKJ+04, LB99, Lip00, MW00, MR07, OY03, Pac06, SPSG08, vRS98, Sta00, TMBM02, WB04a, WXC+05, XWK08, YOL+06, ZOJ+06, ZWB09, Bac04, BG00, BAL+01, BTP09, BMTR01, BZL05, CMSL05, CFS+08, CBC+08, CJS+03, CRH+07, F03, FJ07, FD03, FKE08, Go09, GD09, GPP08, GdAcV+07, GGB07a, KLY03, MCF07, McD03, MHD09, OTL08, OY01, OSA06, Pan07, PMM05, PFMS01, PR04, RG08, SF07, SM03, STCJ08, TD08, Vis02, VZM+08, WSM+09, WOC+03, YT03, YT04, YDWS06, ZZ08, GZG070, ZTP+08, ZM06, WO01].

Computationally [KMO00].

Computations [Bo01, Di05, CLP+05, GP005, Lu09, ME06, POG06, SMZ05, TT08].

compute [BDW00, RKA+09].

computed [PFJ+03, PK05, TDH06].

computer [HFS03, H505, NK01, PX01, PHJ+08, TRS02, UIH09].
Continuous

Contemporary

Contexts

Contributions

Control

Convergence

Convergent

Conversion

Cool

Correspondence

Cor quasi

Cosmo

Cosmo

Core

Core-Excitation

Core-Excited-State

Coulomb

Copper

Coral

Correction

Correctly

Corrector
Coupled [BSP06b, MO01, CXZ+09, DOSG06, IN08, KSTC01, LMJ02, LYS08, PSF+08, SSB07, WKYU01, Whe08, XWC09, SMAdV00]. coupled-cluster [IN08, KSTC01, Whe08].

Couplings [CR08, DXW08, GdAcV+07, KTM02, KBLP09, LB08, MDI04, PJPdPRMI07, QTdG+08, RI08, RLDI09, RRFC+03, SM08a].

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, BA˚A07, CRC+08, CKMC04, FMPS08, LFR+04, MP03b].

Cross [Gan09, MY08b, MY08a].

Crosscorrelation [HWDB03].

Crossed [BAL+01].

Crossing [LI07].

Crossings [LSG06].

Crossover [KRLD09].

Cryogenic [HN02].

Cryotand [WWT08].

Crystal [KOFF09, Van02a, DPT03, EL09, HN02, KP05, TD08, VVVB02, vDSSvA04, vEM01, vE01, DRMD03, FROL08, PZWG+04].

Crystalline [AS00, CADW03, JB04, PZWG+04, Wil01a, ZLD09].

Crystallographic [RON02].

Crystals [BCF+09, CC07, F ´A01a, GAdGM08, GBJ03, PMC+08, RD06, WMS06, Wi01b].

Cs [GWL07].

CSA [NCO+05].

CSOV [GPSP06, PMPGP05].

Cu [BTP09, GPS06, Sha02, HSF08, NK06, TDK07, WMS06, ZTP+08].

CuN [ZK08].

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 [WCS09].

Cyanomethylidyne [WDS06].

Cycle [ZAT07].

Cyclic [KJP+07, BGJ01a, CLA+00, FKM+06, FKM+07, JBGK08, LXL07, OYK+09, VVS07, WOC+03].

Cyclo-AMP [FKM+06, FKM+07].

Cyclization [PWFS01].

Cyclizations [SGS03].

Cyclo [TDK07].

Cycl-Cu [TDK07].

Cycloalkanes [SSBE06].

Cyclobutane [QZZZ03].

Cyclobutene [SRE08].

Cyclohexane [MT03, RP09].

Cycloketones [LLA01b].

Cyclononane [SSBE06].

Cyclononatriene [ZSE08].

Cyclooctatetraene [CPFL02].

Cyclopentadienyl [ML00].

Cyclopentene [SURG06].

Cyclopeptide [FL07].

Cycloreversion [QZZZ03].

CYP2A6 [VB09].

Cysteine [CN05, MOP+07, PMM06].

Cysteine-6 [PMM06].

Cysteines [CFR06].

Cytochrome [AST06, ATBL04, HBM06, JKL08, LCC09, OYH05, OON01, ZAT07, BS06].

Cytosine [KKMMS04, MDA08, MHS05, MH08a, SIB08, SG07a, SC01].

Cytosine-5-acetic [MH08a].

CZ [CRC+08].

D [IS03, PF06, SHBD05, AGO+02, BA+02, CPC+00, DDBP09, DMC05].
FROD08, GDPCPU07, GdSuM+07, GdAcV+07, HP05, LW04b, LXZ06, 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, MPP+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, Adc04, GLD08, KUB07, PSM00]. Dead-end [YFS07, Adc04, GLD08, KUB07, PSM00]. 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, SKDO08, TBSM09, TCR+02, ZZL04]. decompositions [GSP06, PBF07]. decoys [LZ05a, SRC03]. defect [ZMH+09]. defects [JT08]. Definition [dOMSL01]. deformation [GHB04]. deformations [Din00]. deformed [RLER04b]. degenerate [NUH02]. degradation [PCMG09]. degree [CC09, RLER07]. degrees [DHF+05, MZL08]. dehalogenase [NYK+09]. dehydration [TT02]. dehydrogenase [SS05]. dehydrogenases [JH01]. dehydrohalogenation [TT02]. deletion [SHH07]. delineate [MP03a].
delocalization [BY06, BI06, FVB08, FS02, Kar06, GMG07a, GMG07b, WMW03, WW03, WMW04, Van09]. deltorphin [OM04, YAÇ+02]. deMon2k [GJK+06]. denatured [GB04]. dendrimeric [SCG04]. densities [GY08, GBJ03, HSWW00, KCK+08, LMV07, RLR+04, VZVG06, Van02b]. Density [BP01, FG02, Han01, JCHS07, KWK+01, KWK+02, MSBS01, QZ003, QZL+04, VL00, WCW08, AB00, ABYM08, AEE+03, ASY01, Bac09, BP03, BMLV04, BB08, BAA07, CLP+05, CR+08, CFB08, CR08, CSB08, CAG07, CPML08a, Cu04, CGSdT06, DVP+02, DVP+03, DF04, ECM+03, FCW06, FZL07, FDM00, FS04, GLH02, GLR02, GTH04, GTR04, GRY06, GHB04, HGMB04, HLS07, HNW07, HNW12, HNO2, Hir08, Holl05, II02, ION07, IN08, IB04, ITN+05, IS07, JNOV08, Jac09, JCA+02, JFG04, KGL07, KRM+02, KN04, KSS08, KL04, Khi00, KZW+05, Kri09a, Ks01b, LRF+02, Lef06, LV08, LMB08, LMGR05, LLS03, LWH06, LKT04, LF02, LLZL09, LDL+09, LZF+09, MP03a, MV09, MS00, NC06, NTH09, NAT07, OKE+02, PSF+08, RB01, RK04, RLR04b, RDM+08, RR05, RWZ07, SHT07, SZT08, SPT+03, SCF+09]. density [SLRC01, SSB07, SW06, TBB00, TST+08, TKN+08, TKH03, Van02b, VMA03, VBS09, VC04, VKCK09, WR+06, WB07, WZ04, WMRW+01.
WL02, WCH09, WM04, WCL05, WZXY07, WM01, XB08, XL02, XPW09, YTH01, YL09, YK08, YYW07, YLL+09, ZZL04, ZH08, Zho06, ZM03, vGGB00, Haf08, LWK08, MW00, XYN+06, GM01, density-functional [HNWF07, HNWF12, LLS03, LWH06, TST+08, XB08, Haf08]. density/polarization [YL09]. deoxyguanosine [MM02]. deoxyribonucleoside [PFR04b]. deoxyribose [LBG08, SA07].

Dependence [ASS+02, MGLL03, BL00, KH06, NK06, SR09, TJM+03, VKCK09, ZP03, ZXY08, DvG00, DPM09, GM06]. dependencies [FHF01]. dependency [OKH02]. dependent [Bac09, CFK08, FCW06, FCP+04a, Gog08, GS04, HNWF07, HNWF12, HS01, ION07, LDY+08, LDL+09, LSW+01, MML02, MW09, MY08a, NTH09, ONHN00, PSF+08, TST+08, TKN+08, Whe08, WC08, YH07, ZH08, ZM03, vGGB00, PMM05]. 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, KSB09, KS06, KFNH08, MLJ03, SvDS01, TBSM09, WMS06]. Deriving [RPMP03]. desaturation [BBSS06]. descreening [MTE04]. describe [DDBP09, IDMC09, MSH+06b, RLDI09, SBI08]. describing [CM`aGL04, HK08a, HK08b]. Description [ION07, MHT01, BUMCMRL00, BME05, CLWL09, CHRL09, Gri04, HGMB04, SM08a, VMA03]. descriptions [SB08]. descriptor [CDS09, RSS09, TCSM03, XYN+06, ZNL07]. descriptors [AGMPRG+08, BAA07, DA01, EDAJ04, HM08, HMMS09, Jac09, LXW+09, GMGM07b, RUPH06, Tie09, TTB01a, Wou00]. Design [AG03, KV00, BSP06a, BMTSC01, BLMS08, CRH+07, CMBC08, DB06, DHW+07, DHW+09, GHM03, Ham07, HM06, HLTLP09, HLM05, JGVF05, LBFSK07, LZ05b, LFS+07, MWE02, NHH05, PS09a, SPGS08, SRS07, SHM04, STC08, VGGMM05, VZM+08, YFS07, ZZ08, ZL09a]. designed [GT03]. designing [GDV03]. Desirability [CMBC08]. Desirability-based [CMBC08]. desolvation [HMOG07, SVW+05]. Detailed [PB05, WRBV03]. details [GG07a]. detecting [BHH+09]. Detection [WHH+06, BAL+01, CMBC08, OYH09]. determinant [GS09]. determinants [BCP03, Bou00]. Determination [BLT03, CFR06, CR08, DLD+02, FSS00, Vas02, BL08, BR03, BCNs07, BdPRMAI00, CC09, Chi03, CAGR08, FAR02, GCCVB00, HP05, Mar03, MGLDS00, MM07, PC00, PFC03, PABK03, RI07, RTG00, SCF+09, TBSM09, vDSSV04]. determinations [YXL+09]. determine [DDVD09, KUB07, O008, R108, YH06]. determined [OYH05, TDH06]. determining [BY06, DV02, LR06, PHJ+08]. Deterministic [LS05a]. detonation [JWB05]. detoxification [ZWS+09]. developed [CRS05, KMH02, RG08]. Development
Developments [FCP+04b, HS07a, SMD02]. DFT [ASDP+06, ACM+06, BWP07, BPC01, BP07, BSB05, BM08, BB08, BE07, BBSS06, BZL05, CMJ08, CCCJ09, CHA+07, CG06, CS03, CMA+08, DGD+05, Der09, DDBP09, ESP04, EKO+01, EBL+08, FO04, FKŠ+09, GCCVB00, GKH05, GPSP06, GKT504, HT05, HSWW00, HK07, HZ09, Hua09a, JPF+00, Kle02, Kle03, KTM02, Kri09a, KPZK06, LMV07, LYK+04, LSL07, LS08b, LWZ09, LS05b, MML06, MOP+07, MGG06, MBWP03, PFJ+03, PMGP05, PMM06, RM00, SBI08, SWBM08, ˇSBL05, SN06, SCG04, SSBE06, SRB06, Tie09, VS02, VB09, WMGK07, WLX+05, WWT08, WL09b, XLL+02, XKG+05, YK08, 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]. diaminosilylenes [TKS+01]. diamineplatinum [DMN05]. diamond [EKO+01, JBGK08, ZMH+09]. diatomic [ALKH04, FCW06, TLOG00, WWS07]. diatomic [Cal08]. Diatropicity [CdML06]. diazonium [EL06, EL07]. diboran [wQZsLyZ02]. dibromomethane [LXSF08]. dicarboxylic [NHH05]. dication [Bac09]. dichlorides [LHP01]. dichloromethane [RRZa08]. dichroic [MM00]. dichroism [AB08, HKHN08]. didehydropyridine [KC01a]. didehydropyridinium [KC01a]. Dielectric [HS01, DRMD03, GS03, HMWC03, HLMN06, LZZC09, MML02, Vas02, ZFW08]. Diels [Hir08]. DIESEL [ME06]. differ [SRK+00]. difference [ALC08, Bie04a, Bie04b, BF04, PMGP05, PS04, Rud05a, Rud05b, Rud05c, VZM+08]. differences [CV09, GG09, OV03, YZ04]. different [ABA04, BL05, CEP07, CMGDAC+07, DSB+02, MCF07, MN02, VC04, WM01]. differential [DD08]. differently [HSF08]. diffraction [HHJ03, dGWH01]. Diffuse [GS07]. Diffusion [BW04, BZP09, Bie04a, CCCJ09, Rud05a, VW00, PK04]. difluoroethane [CU050]. dihaloethanes [WFR08]. dihedral [FKZ09, HK08c, OFIK09, YL06]. dihydro [WJX+08]. dihydrodiol [PCMG09]. dihydrofolate [GGLR00]. dihydrogen [Mck07b]. Dihydrophospholophosphole [CDL06]. dihydropyridine [HSMT04]. dihydroxypryidine [YXZ+04]. diiminobenzoquinonate [Bac09]. diron [BB08]. diketiminate [GTC06]. diketonate [RMP01]. dilute [HR05, Kri09b, XZ04]. dilution [DA01]. dimension [TSMNG01]. dimensional [BP01, Bie04a, CVR08, DWH+08, LAR+03, LR06, MP03a, MVLG06, RSS09, SHBD05, Wan09]. dimensionality [CDGS09]. dimensions [AHK02]. dimer [CWW09, GYCZ04, Kr030, LJZ03, MHPK01, Mcd03, NK01, RRCA08, SB08, SG07b, YTH01, ZGXX06]. dimerization [HK07, JJK+00, WWX08]. dimers [BB1+09, FKRE08, GYMN07, LMG+09, WLT+04].
dimethoxyethane [LCGA03].

dimethyl [GGGLL05, GWM*00, WLL+03, WJX+08].

dimethyl-2-iodobenzoylphosphonate [GWM*00].
dimethylacetylene [MTB09].
dimethylallenate [ZPL07].
dimethylamin [ZH08].
dimethylcarbamate [KKH+07].
dimethylacetylene [GWM*00].
dimethyl-2-iodobenzoylphosphonate [GWM*00].
dimethylhydrazone [Lu09].
dinitrogen [Ano06a, ST06].
dinicarbonitrile [SMM+08, SDM02].
diodes [LFR07].
diol [Kle02, Kle03].
diol-water [Kle02].
diols [Kle02, Kle03].
dianaphylline [BMRF01].
dioxide [KT08, KZW+05, KK01b, gThDjL01, ZLLS04a].
dioxide-based [KZW+05].
dioxygen [BLO+02, SSW+07].
dipalmitoyl [CEP07].
dipeptide [BISB02, ECA06, HLMR06, JW06, KK09, LRI02, LL07, PFJ+03, Qua07, WD04, YXL+09].
dipeptides [LSW+01, TTB01b, YXL+09].
diphosphates [PFR04b].
dipolar [RI08, San01].
dipole [DVP+02, EDW07, HN02, HK08a, HK08d, HK08b, KFZ03, MLA00].
dipole-quadrupole [HK08a, HK08b].
dipoles [DVRP+03].
discriminant [ZHH09].
discriminants [FTLV01].
discriminating [yCkHmY08].
discrimination [LDTS07, ZPL07].
discriminative [WHH+06].
discussion [CDGS09].
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].
disaccharide [FKJ+01].
disaccharides [SRB02].
DISCO [ZBS03].
DISCOtech [JFG04].

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DNA [AB08, AZM03, BCP03, DLW06, DLVV07, EL06, EL07, FPN+05, FKM+06, FKM+07, JMD+02, JCL05, LW04b, LD05b, LX06, 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].

Docking [NMAT01, ZWB09].

docked [BTLP03, RGZM09, WS02b, AGI+00, AGI+07, AB09, BS05, BS08, CKMC04, CBC+08, CLH+07, CGBF05, CWV+05, CR09b, GZM09, HR08, HLMO5, HW09, KG02, KCL06, LR03a, LDKL05, MKT04, MM03, MCR08, MHL+09, ROK05, RuV07, SBG+09a, TH02, TFN04, TJE03, TP01a, T0t04, VVS07, WRBV03, YK00, Yan04, YKK09].

dodecamer [JCL05].

Does [RY09, RS07a, RS07b, WCK00].

DOIT [SFRS01].

domain [IGNH03, JS07a, OO08, PAT+09, PYCD03, PY05, PC07, PLC08].

domain-averaged [PYCD03, PY05].

domains [GCDL+05, PC05, PC07, SCS07, WCF04].

dominant [LMB08].

DommiMOE [DFWH05].

Donald [Sta00].

donation [HT05].

donor [RM07, SEKS09].

dopamine [FPG+06].

dopants [CM09].

doped [JZGK08, LWLS07, SCP08, WZZ+09, WWL+09].

Doping [SM06, JZGK08].

dot [CLZ+09].

Double [LB05, AZM03, CMJ08, DLRZ09, LMGO+09, Won09, YS00].

double-stranded [AZM03].

doubles [IN08, WKY01, dSVA+09].

doubly [CHRL09, LDL+09].

doubly-linked [CHRL09].

Douglas [YH09].

Douglas-Kroll-Hess [YH09].

downward [LMO09].

DP [CDGS09].

DQ2/DQ7 [KVS+06].

DQ8 [KVS+06].

drag [YSJ09].

Dramatic [AM06a, KT08].

dressed [MW09].

driven [MH09, PV03, SVT09, WPS02].

drives [LFS+07].

driving [AM07].

Drude [LLM09].

drug [CMCB08, DHH+09, HS07b, LWL+09, MCR08, PPXP01, PFR04a, SPGS08].

drug-induced [CMCB08].

DRB09, KEH+02, KC01a, SM0+08, VGGMM05, WM01].

DsBA [CFR06].

Dual [WyLG+09, WLL+03, ZWL+05, mJZlSlyL07, TST+08, ZZL04].

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

Duan [An006c].

due [Car02, JMO7a].

duplexes [BL08, NL08].

duration [CCS00].

during [iza06].

dyad [CHRL09].

dye [BG00, KS05c].

dye-sensitized [KS05c].

Dynamic [SDGC02, XLZ08, CC07, CVR08, CEP07, FEV+09, JW06, mJZlYl+08, LW04a, LDG02, LEV+09, QCK01, QCK02, SDL+09, SCC04, SYC08, WM06, XLC08, YCS07, YCX03].

dynamical [CKW09, EM03a, Kri09b, LDT07, MS03, LPK07].

dynamically [CvG08].

Dynamics [BBG+04, DJB02, KB09, KIM+09, SSBE06, Yos02, ALB09, ATM03, AM06b, BL09, BB05, BBE05, BRDC02, BS01, BG07, CLP09, CLC09, CADW03, CW02, CIB05, CCS00, CF06, CPC+00, CCP04, CMD+04, DLG00, DSS03, DBGV07, ES00, EMP07, ESM06, FSM09, FRRR07, FG02, FBGD06, FEVM01, FKZ09, FNP+06, FPN+05, GL04a, GL04b, Gly06, GS02, GS03, Goo07, GSDT09, GJK00, HB09, HGM04, HSWN01, HNO2, HTSR04,
dynamics
[Maz01, MVL05, MO09, MH08b, MST08, MS01, NK01, NBJ04, NYK09, OO04, OO06, OR05, ON07, PNG06, PRKP05, PMB04, PBW05, Pin01, Pin03, PPYS08, PHH08, PHRR08, PB02, PNG08, QNF09, RRZA08, RMR03, RG08, SO07, SH09, SB08, SBG09a, SLL04a, SM03, STH02, Ste94, SDM09, LWY09, LR03b, Loe03, LMIF06, LM03, LPB03, MB00, MFB04, MN02, MM03, MABM09, MBC08, MCR08, MOP07].

dynamics-quantum [ZSK07].
dynamo [FAB00].
Dyson [SVT09].
E-state [SPGS08].
E1 [YT04].
E2 [RY09].
EADock [GZM09].
early [CMC08].
earth [JHMB09, JHMB11, SO07].
earths [LZZC09].
ECEPP [Sen06].
economic [FZL07].
edge [XWL09].
edge-doped [XWL09].
Edited [Sta00].
Editor [JW12, WM12, vLBBR12, Lip00].
editor-in-chief [Lip00].
Editorial [Bro05].
Editors [BFS07, FA01b, BFS09].
educing [BS01].
Effect [CXZ09, CN05, CEP07, KGL07, Mue01, WMW04, BB08, CP00, CPJ01, CGB09, CSB08, CKT08, DMJ05, GT03, HK08a, HK08b, KT08, KKM07, KCL00, Kri08, Lee09, LL01, LCDA03, Mas04, MZL08, PCS04, RY09, RR05, SOOF05, SPDS01, SCG04, SDL07, VM07, WM06, WDX02, XWL09, ZY01, ZZS07, ZWPR04, CPDZ08, HFS07, JD09, WMW03, WSC09, vE01].
Effective [OCB02, SBLK01, VBGL00, BCF09, CR09a, DPT03, HMWC03, HSWW00, LFK05, MML02, NCTB03, NG04, RPPM03, SG07b, Vas02].
effectively [SMGE08].
Effects [DXW08, KKH07, RLP08, XWX08, AD00, ASS02, BA03, BA04a, BA04b, BPC01, BE07, BDW00, BBI09, CC07, CKF01, CDPL09, Don04, Dra00, ECA06, FGR07, FHF01, GWM08, GVATG03, GM04, GGLR00, GKT04, HRR05, IC08, JJK00, KMM07, KS00, LSF08, LR03b, Loe03, LFR04, MDA08, PBF09, PSF08, PWFS01, RRCA08, SF07, SL09, SMap00, SUG06, SM06, S06b, SRBM06, WSM07, WD04, Wir04, XYN06, YYH04, YH09, ZX04, ZWS02, CM09].
efficiency [KSM05].
Efficiency [IO08, MKGA06, RLR04a, YAC02, CN03, FSM09, GF08, KK08a, L04, LI05, LKW04, PSM05, SM08b, SM03, SE08, vLBBR12].
Efficient [AT02, BP00, BB05, CSJ01, DMZT08, EA08, FL08, FZ09, GH07, GB04, HMWC03, HTKG08, KMA07, KCL00, Nil09, OD09, Oos09, SAT04, SSM08, TP01b, WM12, YZ04, Am00, BL09, BP02, BdPRMA100, CG06, CIB05, CY09, CY13, DBS08, FG02, GJL08, JB00, JB02, K00, LSO04,
LCKL05, PRSMM02, RKA⁺09, SAM06, SSMW09, TS05, Tot04, WW03, YXL⁺09, vLBDR12, FS09, FS00a. efficiently [IGL07, LR06]. eigenvalue [SSL02]. eight [CWV⁺05]. elastic [AJ03, BED02]. Electric [LTV08, SF07, WMS06, ĀCD⁺03, BSOB05, CM09, Kar06, LST08, Mar03, OBBS05].

electrical [KCL00]. electric [LWW⁺06]. electrochemical [Bie04a, Bie04b, Rud05c]. electrocyclization [ZGZX07]. electrolyte [CCCJ09, YSJ09].


electron/four [GYMN07]. electronegativities [dSGCG00].

electronegativity [ALC08, BCNs07, JVK09, VK06].

electrostatic [CCT⁺03, GYMN07, PK05, PML03, RLER04b, SG07b, ABWT09, BCNs07, CPUGD09, CHMI05, DWNB01, FOL⁺04, FY06, GPK05, GB03, KFZ03, KLH⁺04, KCK⁺08, MMPK01, PBM04, PP08b, RL08, SMD00, SFS05, VGDS08, VC04, WCK00, YH06].

electrotopological [SPGS08]. element [Ara04, BHW00, BK08, BH03, BF04, HBW00, HBW01, Li01, SRB06]. elements [ABWT09, ATM⁺07, ASS⁺02, Ell07, JGH00, RP07b, RRS09, VB03, WL04, vW06]. elevated [TK08]. ELF [SFC04, FS00, PC05, PC07]. ELI [BBW⁺08]. ELIA [BBW⁺08]. elimination
Elongation [KLM+09, MKGA06]. Elucidating [DBS07]. elucidation [GZ07, GLH+08]. embedded [CEP07, GGLR00]. embedding [Agr03, JNV08, KS02b]. emission [MLCD01, RGG08]. emitting [LFR07].

Empirical [CBC+08, LS08c, Mac04, SP05, FM00, Gri04, GGK+08, HRKB03, JCHS07, KK08b, LR03a, LLM09, MB00, RKH03, ZNLL07, VBGL+00]. employing [MHT01, THHN01]. empty [CZA03]. enantiomerization [Qua07].

Encapsulated [WL09b]. enclose [ZBS03]. Encyclopedia [vRS98, Lip00].

End [Adc04, GLD08, KUB07, PSDM00, YFS07]. endohedral [KSN01]. endoperoxide [BLO+02, CG08]. enediyne [KC01a]. Energetic [DRAS04, DRAS05, JW12, RP09, BCP03, ECM+03, JD09, KCK+08, PB07, SLHW09].

Energetics [KRLD09, AHGK09, DBGV07, Hua09b, ILKR09, LD05a, MF04, Mas01b, MOP+07, SDCG02, WSC09, ZXY03, ZW09, DLG00].

Energies [CRSB03, BP02, BWE05, BLL+06, BE07, BDW00, CHA+07, CCK01, CPML08a, CG05, DB07, DMZT08, FOL+04, FJP07, FKU+05, GS04, GZL02, GMA04, GLMV09, GAdGM08, GG09, GC04, GS02, GS03, GPSP06, GB02, GWS+02, HKMS01, HP01, HR08, HMOG07, IG02, ILKR09, IGL07, IPN06, IPN07, Jac09, JMD+02, KGN07, KN04, KKC05, KUB07, KB09, Kob03, KCR01b, Kri09a, Lab08, LR03a, LMK01, LF04, LFZ04, LJ04, LB08, LKW04, Lu09, MG06, MCF05, MAF+07, Maz08, MH09, MGAJARC00, MGL003, MRS+07, Nak02, NKIS02, NA06]. energy [OD09, OFB08, OHN00, OKH+02, OV03, Oos09, PSC+01, PMG03, PK04, PAT+09, PMPGP05, Qua01, RP07a, Rao00b, Rap06, RSE07, RRCA08, RWBH09, RLL09, SOOF05, SPDS01, SKGS00, SPL+02, Sch03, SMGE08, Sen06, SRCD03, SMM08, SY09, SG07b, SMMW09, SMD02, SJW09, SSB06, TJE03, TGPP+00, TCR+02, UTH+03, VE09, VM02, Vya01, WL02, WO04, Who08, 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, BSCH+01, EMP07, O006, SM08b, SM03]. ensembles [GLD08, Ik04]. ensure [FKFG08]. enterovirus [KCL06]. Enthalpies [EB04, WC04, BE06, LS05b, RM00, TTBM09, VGGMM05]. enthalpy [OVMV04]. entire [ZAT07]. entropic [CBC+08, FGR07]. entropy [DHF+05, HDF+07, HTKG08, KKH+07, LM03, RK05, Ru07, STSF02, WG02]. enumeration [AL01]. Envelope [BHH+09, BSC+01, EMP07, OO06, SM05, GBL+05]. Enveloping [BHH+09, BSC+01, EMP07, OO06, SM05]. environment [DFWH05, DPM09, GT03, HFS+07, PMM05, GBL+05]. environmental [CMGDAC+07, FGR07, MDA08, TP01a, VW03]. environments [MPF00, ZFW08]. enzymatic [PCMG09]. enzyme [CFER04, Fie02, GGLR00, GS04, MDA08, Pin03, TDH06, VB09, ZL09a]. enzymes [BS06, CPUGD09]. enzymic [CG05, TCR+02]. Epimerization [BBSS06]. Epitope [SHBD05]. epitopes [KVS+06, SHBD05]. epoxide [Owe05]. epoxides [OY01]. epoxy [OY03]. epoxy-amine [OY03]. EPR [SN06]. equalization [BCN07, JY09, VK06]. equation [AMR04, ABWT09, BH00, BH03, BF04, BS07, BS00, BS01, FS00b, Ho05, HBW00, HBW01, SAT04, TW03, Vas02, Vis02, Zho06]. equations [Bi04a, CF04, DOSG06, Ha04, Kv01, LPK07, LMJ02, QNF09, Ru07, Rud05a, Rud05b, Rud05c]. equilibrate [CA07]. Equilibration-Morse [SDCG02]. equilibria [FGR07]. equilibrated [CA07]. Equilibration [SDCG02]. equilibrium [KSTC01, BBP09, ECA06, KBLP09, LS08b, MMLC05, PAS08, ST04, WQK07]. EQUIPATH [Kli]. Equivalent [ZZY07, WBR03, ZZY08]. equivalents [RCJ02a, RM00]. ERE [MCF07]. Erratum [ABBC01a, An05b, An06a, An06b, An06c, BA04b, BRLS12, CY13, FS00a, HNW00, HB01, MK08a, JHM+11, KHS+02, LFS03a, LR03b, NBTO4a, PCO+07a, PW04, RS07a, TZX01b, WB04a, WB05, WMW04, WW+05]. error [IO08, KMA+07, Ko03, Ma04, MD04, RS05, Ru05a, Ru05b, Ru05c]. TB06, VKP+08]. error-ranked [TB06]. errors [CS03]. erythronic [vDSSvA04]. ESFF [SYY+03]. Essay [KHTCG07, FK07b, GR07, Kut07, MGCA07, Nye07, Shin07, Sim07, Tru07]. established [SB01]. ester [TH02]. esters [POJ01]. estimate [KC01b, YZ04]. estimated [ZMZ09]. estimates [GC04, HT05, MD04, SY09]. estimating [DHF+07]. Estimation [DHF+05, ZW09, CV09, DDV09, HLT09, K01b, PYA03, Lab08]. estimators [GZL02]. estrogen [KU05, KBK+01]. ethos [WLG+09]. ethene [Ang]. ether [GLR02, WD04, Y+08]. ethers [ACLD03, LCA03, LCGA03, LCA03, ZYW+09]. ethyl [KKH+07]. Ethylene [TGG00, BSJ01, Hio08, NTH00, SBB02]. Euclidean [RBS09]. EUDOC [PPXP01]. Euler [SG01]. evaluate [GB07a, GB07b, LF04, OS03, TSS07]. evaluated [ABBC01a, ABBC01b, Bo01, Qu01]. evaluating [FO08, Con02]. Evaluation [BML04, DR07, KSM05, NMM01, OYH09, VKP+08, YJS09].
Ano05b, AGSFAL05, CGG06, CAG07, JSR+07, DBS08, ESP04, FMAMVK06, FKZ09, GGA00, HMWC03, JSHG07, KJVV08, KH06, LMV07, LYS08, MSH+06a, Mor02, PRS04, Sha05, VP02, WL02, Yan04, Yas08, CBC+08, GKT04, OGH05, ZSK07. evaluations [SF05]. Evans [SRK+00].

EVEBAT [CZA03]. Even [CVVB04, CC07, VVBV02]. Even-tempered [CVVB04]. evidence [BLO+02, IO08, SFR07]. Evolution [SPL+02, Der09, Mck07a]. Evolutionary [CZA03, LJKL08, QNF09, WL04, AB˚A04]. examples [CMA+08, HBW00, HBW01, SDL+09]. exchange [AAP00, AKN07, BWI+02, EL09, FDM00, GLP08, LMIF06, RRFC+03, SM08a, SM08b, WL04, Wei08, NCO+05]. exchange-correlation [AAP00, EL09, FDM00, WL04]. Excitation [HKHN08, BMB07, Che01, CG08, Hol05, LWZ09, LFEdL06, ON07, PSF+08, SZT08, SA07, SLRC01, XZ04, ZM03, vGGB00]. excitations [DHM+03, ION07, MA09, TJM+03, XZ05, ZX04]. Excited [CHA+07, HFS+07, Ang09, FCW06, FDSA00, HNWF07, HNWF12, IR03, LWX07, LDL+09, MW09, NBTN04a, NBTN04b, NTH09, PO03, PSS+04, SBI08, SMK00, TY03, TKN+08, WLZ07, ZH08]. excited-state [LDL+09, NTH09, PSS+04]. exclusively [RI08]. exercise [FLK+07]. exist [RY09]. existence [WPH+07]. expanding [Bac07, Bie04a, IZA06]. expansion [AHGK09, GS09, GKH05, HTKG08, II02, Ish02, LZZC09, SVDS01, WBSR03, ZFL+05]. expansions [Bou01, DWN01, GC02, JSHG07, RL04b, SG01]. experiment [BE09, GB303, LS05b, Mat03]. experimental [BE06, JARM02, LEK07]. experimentally [KBN02, TDH06]. experiments [CVR08, HP05, OD09, PC00, PFC03, SL04]. Explicit [EC06, PPS08, RI07, AL01, DMJV05, FC06, HM02, JZD+09, KIFK07, KIM+09, LSO04, PK05, RKA+09, WB04a, WB04b, WB05, ZGFL01]. explicit/implicit [LS04]. exploiting [JSHG07]. exploration [CSJ01, HLB09, LXW+09, LM09]. exploratory [PGH+04]. explore [ILKR09]. Explorer [SHBD05]. Exploring [BL05, HPP00, HXL09, KFO8, Sch03, Tie09, SPL+02]. exponent [WTKM06]. exponential [Rud05a, Rud05b, Rud05c]. exponentially [Bie04a]. exponents [MY08b]. exposure [MML02]. expression [dGWH01]. expressions [TN00]. Extended [LMH+09, TVL+03, Bie04b, Cu04, DXW08, KUB07, QNF09, SS00, ST01]. Extending [GCD04, MFB04]. extensible [SYY+03, GBL+05]. Extension [CR09b, FBLO8, GY08, TBGRJ04]. Extensive [JW12, LB08, SLHW09, YXL+09, ZL05, SMG09]. external [CM09, EC06]. extra [LW07]. extra-valence [LW07]. Extracting [HM02]. extraction
extrapolated [KSTC01, Var09]. extrapolation
extrimal [ZZ08]. extremely [GFS05].
Eyring [Nye07].

F
extrapolation [MO09, MC06, PSC+01, PFJ+03]. extremal [ZZ08]. extremely [GFS05].

facility [SWZS04]. factor [LMCD09, WL00, XSHC06]. factorization [EC06]. factors [AST06, SBH02, TP01b]. FACTS [HC08]. family

faster [SF05, AM06a]. faujasite [TLOG00]. faujasite-type [TLOG00]. FB [DHW+09]. FB-QSAR [DHW+09]. FBP28WW [PAT+09]. FDS [TJE03].

field-based [DMLI05]. field-derived [WMS06]. field-induced [CGB03]. fields [ABA04, Car02, EBD+01, HRBKB03, LLM08, Mac04, MFB04, OSHS03, PK04, PB02, RP07a, RLERO4b, RG08, SL09]. files [FJP07]. fill [RRZA08]. find [HQ02, WS07]. Finding [BS01, Qua07, GF08, Rao00b]. fine [VSK+04]. fine-grained [VSK+04]. fingerprints [LHJ+06].

finite [Ell07, MO01, AB09, ALKH04, BHW00, BP01, Bie04a, Bie04b, BF04,
DRMD03, Der09, GM04, HBW00, HBW01, KGD06, PZS04, RP07b, Rud05a, Rud05b, Rud05c, VZM+08. finite-chain [Der09]. finite-difference [Bie04a, Bie04b, Rud05a, Rud05b, Rud05c, VZM+08]. finite-temperature [KGD06]. fire [LDC+07]. First [CS01, HZX04, Hua09b, JD09, JPCA08, KL03, Mck07b, MLJ03, Rud05b, VP08, WLX+05, XYL+09, KSB+02]. finite-order [Rud05b]. First-principle [ZDS+05, GJL+08]. First-principles [CS01, HZX04, Hua09b, JD09, JPCA08, KL03, Mck07b, MLJ03, Rud05b, VP08, WLX+05]. first-row [AD00, BP03, LK03]. fit [BCNs07, SY09]. fitted [YOB+08]. Fitting [KC01b, MCF05, Wei08]. five [SBH02, Van02a]. five-coordinated [SBH02]. fixed [HM06]. fixed-composition [HM06]. Flex [GCD04]. Flexibility [BL08, BCP04, KG02, KTA03, MHL+09, OV03]. Flexible [COS01, NGTB03, YK00, AGI+00, AGI+07, AJ03, AHGK09, BZP09, BTLP03, BS08, CCL06, CKMC04, CLH+07, DDKV07, GCD04, HW09, JNV08, KOFF09, MH08b, SSBE06, TFN04, TP01a, Tot04, VLH+05, vEMK01, vE01, TJE03]. flexible-backbone [AHGK09]. flexible-ligand [HW09]. flexible-protein [HW09]. Flooding [LSG06]. Fluctuating [OR05, KMH02, PB04, PMB04, Yos02]. Fluctuation [MH04, PC05, SBLK01]. fluctuations [AZS+04, WMGK07]. fluid [BCIB05, CLC09]. fluorene [CHA+07, YFR05]. fluorene/pyridine [CHA+07]. fluorene/carbazole [YFR05]. fluorescence [CHA+07, MAF+07]. fluorescent [DHM+03, NAT07, VSW+03, ZI05]. fluoride [BSG07, IV04]. fluorides [KS05a]. fluorinated [CUSS03]. fluorobenzene [ZTP+08]. fluorobutanal [NSB08]. fluorocarbons [JARM02]. fluoroglycine [HS00]. fluoromethylene [ZLL04a]. flux [DAK08, RKA+09, Rud05a, Rud05b, Rud05c]. fly [KMA+07]. FMO [FOK+04, FKL+06, KIM+09]. FO [Gog08]. focal [KK08a]. Fock [RRS07, TW03, WMW04, AKN07, Bon00, Cul04, DD00, AAGM08, HDBD04, MS00, MBWP03, FJ+03, PVdJB00, TYO+02, UHN+09, WMW03, Wei08, YH07, vDSSvA04]. Fock/Kohn [RRS07]. Focus [Mat03]. focusing [KBK+01]. fold [DB06, ZM06]. folded [CP08, GB04]. Folding [HEP+02, ADM+06, CCC03, DG00, HG08, IM06, JS07a, JIK09, KH05, MLG04, MH09, Mei02, MWE02, RSR09, RLP08, VW00, Vw04, VGO+07, ZP03, dSR08]. folds [BS01, ZS04]. following [DDL+02, LMO09]. For-Gly-NH [PC00]. For-L-Ala-NH [PC00]. Force [CLP09, JCL05, OMNH08, OBT09, SO09, SL09, ZWC+09, AM07, AS06, A ACLD03, ABAD4, A006b, A006c, ATBLS04, CLWL09, Car02, CPM03, CLA+00, CR02, CU05, DvG00, DG+04, DW+03, EBD+01, FBDG06, FAR02, FM00, GRO+03, GJG+08, HP01, HGB04, HXL09, HRKKB03, HFS03, HL08, HML07, IDMC09, IT03, IKYM09, JS07b, JM07b, KB02, KSB+02, KS06, KFN08, KTA03, KOFF09, KL03, KTY+08, KL03, KOML08, KDSV02, KVL+04, KBN02, LL08, LL00, LMGO+09, LHI09, LAT05, LH05, LLM09, MT03, MB00, MM05,
Mac04, MFB04, MMLC05, MBC08, MMMY07, MSR04, MRC03, MHJS06, NCO+05, NMTA01, OYH05, OSHS03, ONHN00, OKH+02, OVMV04, PB04, PMB04, PK04, PS09b, PHH+08, POJ01, PB02, PB05, RP07a, RNG03, RI07, RG08, RKH03, SDL+09, SD+G01, SAS05, SDCG02, SF05, SSS+09]. force [SYY+03, SHK+05, SMM08, SK05, TAS07, TTBM09, WZW06, Wil01a, Wil01b, XLT07]. Force-field [CLP09, OBT09, HGMB04, IDMC09, KLB03, MBC08, NCO+05, OKH+02, OVMV04, SP05, VCM01]. forced [CAG07, LPB03]. forcefield [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 [IINK09, Pac06]. formamidine [WJX+08]. format [TDK07]. Formate [ˇCJPZS08, NK06]. Formate-Lyase [ˇCJPZS08]. formates [CUSS03]. Formation [JM07a, RAGLL09a, RAGLL09b, BE06, BMTFR08, CS03, EB04, HIA03, JWB05, Kle02, 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]. formyl [GSB09, HJCP01, FFC03]. formylglycinamide [HRBKB03]. forward [KM07, SJJ+04]. Four [SH02, FJ08, GPSP06, Lai07, PVdJB00, PV03, SBH02]. four- [Lai07, SBH02]. Four-component [SH02, GPSP06, 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 [TT08, XOW+00]. fractional [MGLO03, SM08b]. fragilis [SDM02]. Fragment [DHW+09, CFK08, DPM09, FOK+04, FKL+06, FII+07, FKU+05, FKM+06, FKM+07, IK09, KIFK07, MLG04, MLL08a, NYK+09, NGTB03, NG04, OO08, SG07b, ZMZ09, KIM+09]. Fragment-based [DHW+09]. fragmental [CSB+03]. fragmentation [Go01]. fragments [AM09, DWN01, DPR05, KS01a, LV08, NG04, PBF07]. Framework [JGVF05, CR08, EA08, FS04, TAS07, Tie09]. Framework-based [JGVF05]. Franck [Ama02a, LMCD09, TP01b]. Free [DLRZ09, GS03, JMD+02, MH09, PMGL03, YXC+07, AM06b, BWE05, BLL+06, BCI05, Bli04, CN03, CM09, CY09, CY13, Chi03, CV09, CCK01, CMGDA+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+09, KKC05, KUB07, KB09, Kob03, KK01a, Lab08, LR03a, LF04, LSW+01, LKW04, MG06, MT03, MGL003, MRS+07, OD09, ONHN00, OKH+02, OV03, OVMV04, Oos09, PK04, PAT+09, RSE07, RWBH09, SOOF05, SAM06, SKGS00, STSF02, SBL05,
glycol [Pin01, RR05].
glycol-lesioned [Pin01].
glycosidase [BMTFR08].
glycosidase-inhibitor [BMTFR08].
glycosidase-substrate [BMTFR08].
glycosidic [SO09, SDL+09].
glycosidase [BMTFR08].
glycosidase-substrate [BMTFR08].
glycosidic [SO09, SDL+09].
glycyl [KOML08].
glycine [CCK01].
gold [BR04, CZ05].
gold-capped [CZ05].
GolP [IDMC09].
good [VGGMM05].
GPCR [XWC09].
GPCR-CA [XWC09].
GPU [NYTH09].
Gradient [SE07, DLD+02, JSR+07, FRLN09, GMA04, ION07, Ish02, IPN07, LST08, TNS00, WL02].
gradient-based [FRLN09].
Gradients [WM12, BWP07, HHS+05, IK00, KBT03, LJ04, SSMW09, vLBBR12].
grain [PSHP08].
grained [CP09, DR07, DJB02, HXL09, MBC08, SBJ08, VSJ+04, VTT+08, WWL+09].
graining [CA07a, EBAN07].
grand [EMP07].
GRAPe [Höf05].
graph [CLZX09, MGMM07a, Pog03].
graphene [KK08c].
Graphical [BMTFR08].
graphically [GS09].
graphics [FEV+09, SPF+07, Yas08].
graphite [BCF+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, THHN01].
PRSMM03, PV07, RFSS06, RWBH09, SOOF05, SEKS09, SLL+04a, WDS06, WTKM06, Wei08, Wil01b, WDX+02, YTY07, ZY01. H-bonded
[LB05, McD08, NL08]. H-NMR [AGI+07]. H5N1 [DLRZ09]. Hairpin
[ZHH09, CJW+09, IGN03, LHI09]. Hairpins [IGN03, Der00]. Half
[FMAMVK06, PS03, PMM06]. Half-numerical [FMAMVK06].
half-reaction [PS03, PMM06]. halide [RC04, CW02]. halides
[AB00, LYK+04, LSY02, ZJM+07]. Hall [SPGS08]. halo [TT02].
halo-hydroxyformaldoxime [TT02]. haloacid [NYK+09]. haloalkane
[CS03]. halogen [BS03, FHF+01, GGP09, LZF+09]. halogen-bonded
[LZF+09]. halogenated [STC+08, TZX01b, TZX01a]. halogens [TBGRJ04].
halothane [TZX01b, TZX01a]. Hamiltonian
[FRG07, FBL08, MR02, SAM06, ZWPR+04]. Hamiltonians [CV09]. hand
[DFGB09]. handle [GCD04, GM04]. Hansen [BBG+04]. Haptic [MR09].
hand [TGP+00, ZHMW09]. hardness [PRS04, TSSGS07, TSSSG08].
hardware [ATMK03]. harmonic [CLP+05, Ish02, TFN04]. Harris [Cul04].
Hartree [WMW04, AKN07, Bou00, Cul04, DD00, GAdGM08, MS00, MBWP03, PJF+03, RSS07, WMW03, Wei08, YH07]. HAsXH [L508a].
having [WJ00]. haystack [BS01]. HBCC [BAL+01]. HBOP [OYH09].
HBr [SLL+04b]. HBSITE [OYH09]. HCCX [Mar03]. HCl [BL06, WDS06].
HCO [JPF+00, dRLMS00]. HCO-L-SER-NH [JPF+00]. HDMR
[LRWG03, LAR+03, LSHR04]. head [HSWN01]. heart [TKH07]. heartland
[Sha07]. heart [DMSL01]. heats [CS03, JWB05, RCJ02a, WX09, LLA01c].
houer [ZJM+07]. heavy [BPC01, WL04, ZX08]. heavy-metal [ZX08].
HeC [Var09]. Helical
[CPML08b, Van08, Der00, KF02a, LC09, PCO+07b, PCO+07a, ZALMG03].
helicenes [VKP+08]. helices [IGN03]. Helix
[BRDC02, JS07b, LI07, PP08a, YS00]. Hellmann [RLER07].
hemagglutinin [DLRZ09]. heme
[ATBLS04, MBM+00, OYH05, RGZM09, RZWS07]. hemicarcerand
[LMMW04]. hemoglobin [MML+06, SO07, Sen06]. Henry
[Sch00, TLOG00]. hept [STC+08]. hept-C [STC+08]. heptafluoropropane
[LDC+07]. heptagon [STC+08]. heptagon-containing [STC+08].
heptapeptide [OM04, YAÇ+02]. herbicidal [XYN+06]. hERG [MCR08].
Hess [YH09]. Hessian [KK01a, NKls02]. Hessian-free [KK01a]. Hesians
[ASLG07, Cha07]. heteroaromatic [LLM09]. heterobimetallic [RD00].
heterochiral [ZOJ+06]. heterocycles [FSS00, MGMM07b].
heterofluorines [CZFH07]. heterogeneity [HS01, ZSC05]. heterogeneous
[FCF+08, ZCS04]. heterohelicenes [LC09]. heterolevel [EA08].
heteropentalenes [CDL06]. heteropolymers [SBJ08]. Heuristic
[DMC05, DLHC06, CAGR08, IZA06]. Heusler [GD09, KGD06]. hexadiene
[PA05]. hexadiyne [PWFS01]. hexagonal [BK08, LTF+07]. Hexahelicene
[LC09]. hexamer [NK01]. hexatrienaldehyde [ZGZX07]. hexopyranose
[GGK+08, LH05]. hexopyranose-based [LH05]. HF
[BRLS12, BRLS08, FKJ+01, GKTS04, PMPGP05, WW03]. HF/6 [FKJ+01].
HF/6-31G* [FKJ+01], HF/DFT [BRLS12, BRLS08], HF/MP2 [GKT04], HF/CO [JHPRSM+05], Hg [GPS06, BBI+09, WTKM06], HH [CMaGL+04], HI [KKJH08], Hiberty [Bi09], hidden [FWH+07, HLT+05, RP07a], hierarchic [RRS07], Hierarchical [LMH+09, CWV+05, DJB02, FOK+04, LCC09, UIHN09], High [BB08, GAdGM08, LAR+03, AZM03, BACJC01, CCWH02, CN05, DPT03, GL04a, GY08, HGMB04, JBB00, JBB02, KWK+00, KVF+00, LR06, Mck07a, Mck07b, MTB09, RP07c, RLER07, RSS09, SSS+09, WMRW+01, WS05b, XK08, UTM+02], High-dimensional [LAR+03, LR06, RSS09], high-latency [KVF+07], high-level [WS05b], high-performance [CCWH02, KWK+00], High-precision [GAdGM08], high-quality [JBJB00, JJB02, SSS+09], high-rank [RP07c], high-resolution [GL04a, WMRW+01], High-spin [BB08, DPT03, Mck07a, Mck07b], high-valent [AZM03, CN05], higher [BF04, HTN03, WRP+06, ZSK07, AAP00, BBSS06, DMN03, DDBP09, FAR02, FAB+00, FMSA06, GRO+03, GLD08, HBB00, Han01, ION07, JPCA08, JJK09, KRM+02, KN04, LS05b, LW09, LS05b, MBM+00, MS+06a, PDS01, RDM+08, Sza08, THHN01, TFN04, WWL+09, XLZ08, ZZL04], Hybridized [SJJ+04], hybrid [GXK09, Kan07], hydrate [ME02], hydrated [ITS05, XT04, YS09], hydrates [EM03a], Hydration [BZL05, CFC+08, HNO2, BLB+06, CMD+04, GZL02, HB09, HKMS01, HM02, Lab08, LSW+01, MS03, NTH00, OVMV04, PK04, Pin01, RSP03, UBDPJ04, XLT07], hydration-parametrized [RSP03], hydrazines [BLN01], hydrazine [Lu09], Hydride [GVATG03, JHJ01, LLXS02], hydrides [KS01b, SRB06, dSGCG00], hydridotris [HT05], hydridans [HKHN08], hydrocarbon [CS01, KFD06, LC06, Wan09, WEE01], hydrocarbons
Hydrodynamic [BZP09]. Hydrogen [Bor03, BS03, EB04, FVB08, LS08c, MGMM07a, SDvG01, VS08, WFHP01, WJ00, ZKZ+07]. Hydrogen-abstraction [WLLS04]. Hydrogen-bond [RM07, SPT+03]. Hydrogen-bonded [CPDZH08, LDL+09, MH08a, ZH08, vEMK01, vE01]. Hydrogen-bonding [AG00, ZW09, Yos02]. Hydrogenase [TDH06]. Hydrolases [OBT09]. Hydrolyses [DWS+09, LYK+04]. Hydrolysis [WOC+03, DLR+08, MBL+00, RP04, TH02, WJX+08]. Hydroperoxy [BL06]. Hydrophilicity [DLHC06]. Hydrophobic [MBH+02, CJDK09, HJC01, SDL07]. Hydroxide [CBS+03]. Hydroxyl [CUS00]. Hydroxylase [HLC09]. Hydroxymatairesinol [SH09]. Hydroxyproline [WXX03]. Hydroxyaromatic [BLO+02]. Hydroxyformaldoxime [TT02]. Hydroxyformaldehyde [DKZ09]. Hydroxyl [CUS00]. Hypochlorous [JKM08]. Hypersurface [PSC+01]. Hypersurfaces [PSC+01]. Hypochlorous [JKM08]. Hypothetical [LD05a]. Hypoxanthine-cytosine [KKMMS04]. Hypoxanthine [KKMMS04].
NBJ04, PZWG+04, SAM06, SM08b, TT01, VK06, WCC08, YCYXY03, LLL03, VV03, YOB+08. implementations [FL08]. implemented [HP01, MP03b]. implementing [OR05]. Implications [Ano06a, JS07b, KS05c, NHH05, ST06]. implicit [BBHD04, BLL+06, GL04a, JS07a, JZD+09, KTA03, Kr063, Lab08, MCM04, PZ04, PPS08, SBLK01, SL06, WL09a, ZGFL01]. Importance [CGBF05, ENM+04, ZM06, HLC09, JW06, OCB02, PMPGP05, PMM05, TS05]. important [CSU05, EDAJ04, Tor02]. improper [TNS00]. improve [FSM09, XLT07]. Improved [CN03, CLA+00, Gri03, HQ02, KK08a, KK08b, LK04, RCJ02a, SKSH07, TGD05, Wil01a, Wil01b, CMBC08, JRS+07, KDSV02, MP03b, Maz08, MFR07, PABK03, PRS04, SD+G01, STSF02, SH+05, VZM+08, LK03, RCJ02b]. Improvement [SM08b, UKN04, Nee03]. improves [CLWL09, RK05]. Improving [BUCMRL00, Bie04b, GF08, LJ04, LKW04, GRO+03, GP06, SMG09]. in-core [FR06]. inactivation [PFR04a]. incidence [YWHZ03]. InCl [ZL05]. Including [IC08, AKN07, DP03, DP04, Gri04, Ish03, LB08, SL09, Wil01a]. Inclusion [HK08a, HK08b, PWHF+03, PWHF+04]. incomplete [FHW+07, Ish04]. incompressible [ZHMW09]. incorporate [KTA03]. Incorporating [CLS+09, DJM05, HLT+05, SL+09, HS01, LL07, RD06]. incorporation [SM06]. Increasing [ZWZ09, BT00, LJS05, YA+02]. independent [FV08, OTL08, Van02a]. index [COS01, JH03, MBH+02, PVdB00, Pog03, YWHZ03, YWH04, YYW07]. indexing [HWDB03]. indicators [BW+08, HIM07]. indices [BLT03, CGMPT+08, FZL07, FMP08, FVB08, FS04, GDPCPU07, MGM07a, MGM07b, May07, Rao00a, SPGS08, TSMG01, TSSG08, WMW03, WW03, WMM04]. indium [ZL05]. individual [ZM06]. INDO [PBZ00, TY03]. INDO/SCI [TY03]. indole [LL01]. induced [CGB03, CMBC08, 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 [GBS09, JS07a, JT08, LZA02, BGC+09, SBH02, SLRC01, DB06, EL09]. Information [Ham07, GCB03, HTKG08, HP05, NL08]. information-bearing [NL08]. infrared [CVR08, Kle03, LDL+09, MGLD00, TDH06, Zer08]. Inherent [BYQS03]. inhibition [PFR04b, WC08]. Inhibitor [VV07, BMTFR08, CWV+05, FPG+06, MBC08, SVV+08]. inhibitors [AJNG01, AGO+02, APG05, AVS09, LLL+08, LZ05b, PB06, RGP+07, VBG09, VVS07, WZY04, WH08, ZWB09]. inhibitory [DD08]. inhomogeneous [MZL08]. initial [MM03, MABM09, Qua07, UNM+01]. initialization [FKFG08]. initiated [RAGL09b]. initiation [GGGLL05]. initio [AJ03, Ama02a, Ama02b, An006b, ASY01, BG03, BG00, BL08, BSB05, BS01, BL06, BLO+02, BSJ01, BZL05, CPJ00, CPM03, CUS00, CU01, CUSS03,
GGP09, Gon07, HLC09, HA04, HZ06a, HZ06b, IINK09, IB04, JWB05, KF02b, KH06, LHI+06, LCC09, LZ03, LS08c, MM05, MMLC05, MCF07, NK06, Nil09, PG01, PC0+07b, PC0+07a, PK05, PNG08, RZWS07, SOOF05, San01, Sha05, SSS+09, SWV+05, SG01, SL06, SDL07, SMV+09, UTT+04, VW03, WR+06, WPH07, Won09, YT03, YTH+07, ZTS09]. interactive
[DFGB09]. interactively [SB01]. Interatomic
[RD06, AMR04, SS00, SPT07]. interconnected [SB08]. Interconversion
[OO04]. interconversions [FD03]. Interesting [Kri09a]. interface
[CF04, DPDG05, FOK+04, GRR08, HHBH00, HZX04, JKI08, KKG+09, LLL03, LPB03, PHJ+08, 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, BMTR08, IGNH03, MMMY07, OBTO9, WSM+09]. Intermolecular [PSC+01, AS00, CMAGL+04, CLC09, FA01a, FMK+06, FMK+07, GGP09, GS04, IGL07, KS05c, LZJ03, Mas04, MPMGP05, RRCA08, SPDS01, SJW09, UTM+02, UTT+04, Wil01a, Wil01b, ZDS+05]. Internal
[EA06, BHH+09, CFD03, CFD04, COMR+04, DHF+05, Din00, HFSD03, KS03, KTA03, LKP07, MGLL03, NKIS02, SWO06, TNS00, WR07, WFR08]. internal-rotation [DHF+05]. interparticle [PK05]. Interplay
[EFQD09, SP05]. interpolated [YK08]. interpolation [BB05, IS03]. interpretation [CPJ00, HLS07, VM07]. intersection [SSHT03]. intersections [IK00]. interval [LS05a]. interwall [ZZRSC08]. Intra
[FA01a, FMK+06, FMK+07, MAF+07]. Intra- [FA01a, FMK+06, FMK+07]. intraphycocyanin [MAF+07]. Intramolecular [GKT05, HA04, PG01, TFZRG01, AGK03, BA03, BA04a, FDS00, HRKB03, HK08d, LI01, NHH05, RP02, SWV+05, VIP+06, ZDS+05, ZW09, ZH08, KLE02]. Intraprotein [MLJ03]. intraresidue [IB04]. intrinsic
[JS07, JT08, YGZZ05]. intrinsically [NAT07]. Intruder
[CWY09, WCFH02]. intuitive [PP08b]. invariant [Est07, ZLY07]. Inverse
[BR03, MLL08a, Ni09]. inversion [KSTC01, RC04, ZSE08]. investigate
[DWN01]. investigated [HN02, KLE03, YH09]. Investigation
[LZZC09, YTH01, AST06, BL00, CW02, CHA+07, CG08, FG03, GS04, Hir08, JH01, KYFW07, LH02, LXS08, NSB08, PV07, QZZZ03, QZL+04, RM07, RC04, RY09, SL04, TGGP+00, TFZRG01, UCT+03, WL09b, WLZ+07, ZXY08, ZKZ+07, ZHWM09, ZGZX07, GBJ03, JBGK08]. Investigations
[JP09, WG02]. involvement [BLO+02]. involving [LL01, MM05, ZGZX07]. iodides [CM09]. iodine [GWM+00]. iodobenzoylphosphonate
[GWM+00]. Ion [DAK08, BM08, DRa00, EL07, FHR07, FL07, GWM08, Gor01, ISV06, KPR04, Kri08, Kri09b, MSB01, PPS08, PHRR08, RC04, VHR07a, VHRR07b, ZZW09, dOMSL01]. ion-pair [RC04]. ionic [Ang09, BM08, BS07, BGJ01a, CFC+08, DJV05, GGT08, HTN03, LR03b, LOE03]. ionizable [OS06]. ionization [GSB09, KFD06, RTG00, SVT09]. ionospheric [LSHR04]. ions
[CXZ +09, DMJV05, EL06, FG03, HTSR04, HLB09, JRJ01, KT08, KZRO03, LSWB00, LMIF06, MHS05, RMP01, SL09, ZSC05, ZZZ +06]. IPR [GZ07]. IR [NRKH02, ZWTP +08]. iron [DPT03, GK09, HLLN06, IWH06, MSH +06b, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06]. iron-containing [MSH +06b]. irregular [ZBS03]. irrelevance [VVBV02].

ISBN [Bic09, Lip00, Sta00]. ISBN-10 [Bic09]. Iso [GWL07, Rap06]. Iso-energy [DPT03, GK09, HLLN06, MSH +06b, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06]. Iso-guanine [GWL07]. isobaric [SM03, Ste04]. isocyanates [OY01]. isocyanide [HT05]. isocyanurates [OY01]. isoelectronic [Che01]. irrelevance [VVBV02].

iso-energy [GWL07, Rap06]. Iso-guanine [GWL07]. Iso-energy [Bic09, Lip00, Sta00]. ISBN-10 [Bic09]. Iso [GWL07, Rap06]. Iso-energy [DPT03, GK09, HLLN06, LWH06, MSH +06b, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06]. Iron [DPT03, GK09, HLLN06, MG06, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06]. Iron-containing [MSH +06b]. Iron [DPT03, GK09, HLLN06, MG06, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06]. Iron-containing [MSH +06b]. Iron [DPT03, GK09, HLLN06, MG06, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06]. Iron-containing [MSH +06b]. Iron [DPT03, GK09, HLLN06, MG06, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06]. Iron-containing [MSH +06b].
L

[47]

L-2-haloacid [NYK+09]. L-captopril [AGO+02]. L-peptides [OYK+09]. L-phenylalaninamide [HJCP01]. L-valinamide [HJCP01]. L/SSB [KVS+06]. label [VCM01]. lactamase [AGO+02, APO05, SDM02]. lactamases [ESM06, MK02]. LADH [DMC05]. La [VP08]. 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, BdpMaj00, BME05, CJK+02, CDD+02, CG06, DMN03, DJB02, Ell07, FZL07, HB09, HSM06, IME02, IS07, JO02, JW00, KS05b, KKG+09, KK01a, KH06, LMJ02, MKGA06, MH09, MHW04, MH08b, MPF00, ME06, NRK02, PFJ+03, RRS07, SYC08, SSL02, TYO+02, VSK+04, WWL+09, YCS07, vGGB00, WS07]. large-amplitude [KS05b]. Large-scale [WCF04, DMN03, JO02, KK01a, MH09, MHW04, MPF00, ME06, RRS07, SSL02, TYO+02], larger [VKP+08]. lariat [ZWY+09]. LCAO [EBL+08, EL09]. LDA [RLD09]. lead [RS07a, RS07b]. leads [PPX01]. learning [YCW+09]. least [CSD05, Gol09, LLZL09]. least-square [LLZL09]. LEDO [GKH05]. legacy [Sha07]. Lei [Ane06c]. length [CRC+08, DR09, JPCA08]. length-frequency [DR09]. lengths [PSC+01]. Lennard [CYM02, FSF05, Pul05, SCC04, SYC08, YCS07]. Lennard-Jones [CYM02, FSF05, Pul05, SCC04, SYC08, YCS07]. lesion [Pin01, Sh08]. 8esionized [Pin01, Pin03]. Letter [BFS07]. Letters [JW12, WM12, vLBMR12]. level [Bumcmrl00, BLT03, BL00, DPM09, JMD+02, mJzlsLy07, KK08c, PFJ+03, RC04, TBG00, TST+08, UTM+02, WyLG+09, WS05b, WLL+03, ZZL04, ZWL+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, Lwk08, Lww+06, LAT05, WWT08]. libraries [AL01, KV00, LZ05b, ZM09]. library [CRI+07, FAB+00, Kms05, OTL08, Sh07]. LiF [EL09, UM03]. lifetime [CHA+07]. Ligand [MKT04, AM06b, Bsp06b, BGC+09, BS08, BMTsc01, CGB+09, CLH+07, CN05, DFWH05, F008, GZM09, HZ06a, HZ06b, HW09, Jzd+09, Ks08, Lxw+09, Mue01, N04, Nmat01, OFIK09, PWHF+03, PWHF+04, RK05, Ruv07, SOO05, STSF02, TFN04, Tje03, Vgmm05, XZ04, YK00, Yan04, ZfgL01, ZWS+02, BDW00, HLC09]. ligand-charge [Bsp06b]. ligand-protein [Vgmm05]. ligands [Jvk09]. Kr [CMJ08, CGB03]. Kroll [YH09]. Krylov [Har04]. krypton [CVVB04].
M [Bof01, GPSP06, JJK+00, LYZ+08, OS08, Qua01, WWC+05, JJK+00, LMGR06, OS08]. machine [CLS+09, HL08, LIZ+07, YCW+09]. machines [CLXC02, QLHL09, YMT04]. macro [Wou00]. macromolecule [RRZA08]. macromolecular [FLOD07]. Macro cyclic [SCG04, KB02]. macromolecular [Ara04, Con02, EA06, FM00, JO02, KS01a, KHY00, RP07d, ZBS03]. macrocycles [BM08, HL08, LJZ+07, YCW+09]. micro [CLXC02, QLHL09, YMT04]. macrocycles [FLOD07]. Macrocyclic [Wou00]. macrocycles [CLXC02, QLHL09, YMT04]. Macrocycles [RRZA08]. macrocycle [SCG04, KB02]. macrocyclic [Wou00]. magnetism [Hua09b]. magnetizability [YH07, YH09]. magnetizabilities [YH07, YH09]. magnesium [ZZW09]. magnetic [BACJCT01, CDL06, CDPL09, DXW08, HWFN01, HIM07, KCL00, KGD06, MV06, MD04, PJPJPRMI07, QTdG+08, RLDI09, TDK07, WZXY07, ZPL07, ZXY08]. magnetization [Hua09b]. magnetization [Hua09b]. magnetization [Hua09b]. magneto- [BACJCT01]. main [Din00, JGH00, LW07]. main-chain [Din00]. maingroup [SRB06]. main-group [SRB06]. Maintaining [LFBSK07]. maleimide [RP09]. malonyl [LLL+08]. malonyl-CoA [LLL+08]. maltose [MW00]. maltotriose [SWBM08]. Manager [FCK+08]. manganese [AZM03, CWY09, GK09, LMIF06, LS05b, RJLR06]. Many [Loe03, BM08, TKH07, YCXY03, LR03b]. Many-body [Loe03, TKH07, LR03b]. many-electron [YCXY03]. map [MLL08a, SKGS00, HLTLP09]. mapping [FKZ09, RL01]. maps [PRT+07, PRT+08, TTB01b, WD04]. Marchi [Ano06b]. Marcus [BNL01]. Markov [BHG03, CPUG09, CMGDAC+07, DLW06, FWH+07, HLT+05, SK09]. Markovian [YCXY03]. mass [GM04, Gor01, KZW+05, LHZ+06, ZWZ09]. masses [CN03]. Massimo [Ano06b]. Massive [TP01a, RL01]. massively [DGHR02]. master [FR06, FS00b]. master-slave [FR06]. matching [SMM+08, VSW+03]. Material [JW12, SLH09]. materials [BCF+09, Haf08, LLXS02, LMRVF09, Tie09, XXY08, YPNE09]. mathematical [DDVD09]. matrices [AT02, BDPRAI00, CZA03, LSAS01]. matrix [CGSdST06, Ell07, GHH07, IS07, JCA+02, Li01, NKIS02, Nee03, RS05, RRS07, RRS09, SK09, SSS+03, TYO+02, UHNN09, YWZH03, vDSSvA04, vW06]. Matteo [Ano06b]. matter [ASDP+06]. maxima [MSH+06a]. Maximal [GCDL+05]. maximization [BW1+02]. maximizing [AM07]. Maximum [MWE02, SCS07, HXD08]. MBO [CPC+00]. MC [HMD06, MLG04]. MCCd [SMG09]. MCDP [LAEL01]. McLafferty [NSB08]. MCM [NCO+05]. MCPRO [JTR05]. MCSF [IR03]. MD [KIM+09, MDA08, ALB09, BMRF01, CADW03, HRR05, H05, PHR08, WRBV03]. MD-based [BMRF01]. MD-GRAPE-2 [H05]. MDGRAPE [KAK+09, NYTH09]. MDGRAPE-3 [KAK+09, NYTH09]. MDSimAid [CHM10]. mean [GMA04, HFSD03, LHI09, MMLC05, NMA04, RNG03, YCXY03]. meaningful [AE06, Bu07]. means
measure [XSHC06, ZHH09, PDC+08]. measurement [YZ04]. measurements [KBLP09]. measures [BDW00, DW08, Ham07, Leh06, PYEA03, PCA+08, PDC+08]. mechanical [AVB00, BISB02, CLP09, CGBF05, CCK01, COL+06, DWC+03, ECA06, ESM06, EBD+01, FHR07, FÁ01a, FAB+00, FKU+05, GAIMVB01, GGLR00, JJH01, KKS04, MP03a, MBL+00, Sau04, TCR+02, VHRR07a, VHRR07b, XZZ04, XLZ08, YPNE09, ZCZ03, ZAT07]. mechanical/molecular [CGBF05, FÁ01a, TCR+02, VHRR07a, VHRR07b, XLZ08, ZAT07]. mechanics [AS06, AS09, AD00, AM06b, AGO+02, APG05, BDW00, CLFA07, CR02, CSU05, DPT03, DFWH05, DWC+03, EC06, FEVM01, GCD+08, GS04, GKT04, GPK05, HWTL03, JČHS07, KL03, KZRO03, LL00, LLA01a, LL01, LLA01c, LL01d, LLA03, LSWB00, MLA00, MFB04, MPF00, OSIS03, PRKP05, PS09b, PWHF+03, PWHF+04, RMP01, RSE07, RP02, RO00, RM00, RGP+07, SS00, SH+08, TG+00, TFZR01, TT05, VSW+03, XOW+00, YSA+03, ZSK07]. mechanics-based [BDW00, RSE07]. mechanics/molecular [MPF00]. Mechanism [CJK+02, LWY+09, PFR04a, Rao00a, AM07, AGK03, BTP09, BLO+02, BS03, CGB+09, CBS+03, DBS07, HP04, HLB09, mJZsLyL07, JDWS06, JHH01, LMGO+09, LPP06, LL01, LDT+02a, LDT+02b, LYZ+08, LFS+07, MCK05, Mui05, PGN03, PFR04b, PS03, PMM06, wQZsLyZ02, QZZZ03, RJJ06, SMKM00, gThDjL+01, WDWS06, WCHW09, WXX03, WJX+08, YQQH09, ZLS04b, ZLS04a, ZLS05, ZLS06b, ZKZ+07, ZGZX07, GVATG03]. mechanism-based [PFR04b]. mechanisms [AGI+00, AGI+07, BS06, CCCJ09, CG05, ILKR09, KZY09, KJHK08, LLL06, M02, NSB08, RC04, SIE01, TMBM02]. Mechanistic [BMTFR08, SG03, TT02, An06a, ST06, WD06, XDS06a, ZLS06a]. media [HLLN06, MM02, SMKM00]. mediated [HIA03]. medium [FZL+06, HXLS09, LF04, LFZS04, SHH07, ZFL+05]. medium-resolution [HXL509]. medium-sized [SHH07]. melatonin [CKT+08]. mellitus [PS09a]. Melting [LML+00, KT02]. membered [FJ08, ZW09]. membrane [ALB09, CJDK09, DAK08, FCP+04a, GAS04, ILKR09, JMO7b, LPB03, MJJS06]. membranes [Ie04, SSM08, WC09]. memoriam [Ano00]. memories [WHRG08]. memory [TYO+02]. mercaptocarboxamides [TFZRG01]. mercaptocarboxylate [APG05]. mercaptopyridine [YXZ+04]. mercury [FNP+06]. Merging [PPJ07]. Merz [JVVK09]. Merz-Kollman-Singh [JVVK09]. mesh [BYQS03, KM00, KSY+00]. mesoscale [RPMP03, ZBS03]. Mesoscopic [YPNE09]. Met-enkephalin [ZCL09]. meta [DDBP09, ION07, ZTP+08, Gan09]. meta-di- fluorobenzene [ZTP+08]. meta-generalized [ION07]. metabolites [PCMG09]. metabolizing [VB09]. metabotropic [FTLV01]. metadynamics [BBP09]. Metal [SGD06, ABYM08, An06a, Bac05, BTP09, BS06, BRV+07, BM00, BWI+02,
metal-catalyzed [HSWW00]. metal-free [CM09]. metal-organic [TAS07].

metal-porphyrins [LS02]. metal-rich [LWK08]. metallic [ALC08, KWK01, KWK02, SK08, WLX05a, dVB01]. metallo [AGO02, APG05]. metalloenzyme [BSDM04]. metalloenzymes [Sie01]. metallofullerene [CTFC08, KJP07]. metallofullerenes [KSN01]. metalloproteins [CR09b, SN06].

metals [BP03, BGJ01b, CM09, LD05a, LK03, LK04, WLX05b]. methanediamines [CPJ01]. methanol [CCK01, YGLvG06, ZH08, ZWP08]. methionine [BTP09].

Method [KFB05, MO01, YGZ05, AK07, AB04, AE06, Am00, ATM03, AB09, A005b, A04, BL09, BW07, BP01, BW04, BCN07, Bie04b, BH03, BF04, BM00, BGC09, BHG03, BHH09, CC09, CCL06, CSJ01, CG03, yChHmY08, CRG01, CPC00, CAG07, CA04, DPT03, DMRD03, DPRR05, DMLI05, DVM09, ECM03, FOK04, FKL06, FII07, FÁ01a, FAR02, FS00b, FSL09, FKL05, GMA04, GS09, GY06, GB04, HD04, Har04, HFS07, HH05, HSWF07, HNWF12, HQ02, HFD07, HSWW00, I09, IR03, IK00, JO02, JVV09, K01, KD09, K04, KTA03, KN04, KM00, KLS02, KKC05, KSY00, KK08a, KOL04, KIM09, KB09, KLM09, KC01b, LS00, LRW03, LR06, LWX07, LZZC09, LWX09, LCS09, L05b, MLL06, MKGA06, MKT04, MB00, MCF05, MS06a, MH08b, MG00, MS01, MY08b]. method [MPF00, MRS07, N005b, N006, NGT03, NG04, Nye07, OM04, PHJ08, PAK03, PMC08, PZ04, Qua07, RGO03, Ra00b, RSE07, RL04, RK05, SK09, SMAD00, Sch04, SCC04, SYC08, Sha05, SF05, SG07a, SW04, SV09, THH01, TN04, TVL03, TY03, TK08, VP06, VZ08, VM00, Vya01, WS00, WW03, WLZ07, WL00, WBS03, WM04, WX09, XL02, Yan04, YZ06, YCS07, YAČ02, YH06, YM09, YX09, YXL09, ZWS02, ZL09a, vVGD00, JB00, KTM02, SRC03]. method-based [KIM09]. methodological [FDAS00, MFR07]. Methodology [KS02a, SPL02]. Methods [SB01, AJ03, AGMPR08, BB05, BL05, CAM08, CG05, DLD02, DB07, DMM03, DB03, DHRD09, FOL04, FO08, GHLK02, GH07, GY08, GD09, GPN01, GGLR00, GHBB04, HTKG08, IB04, JFG04, KK08a, KBL08, KLE02, KLE03, KB09, LM07, LMB08, LL03, LW06, LHP01, LK03, LKW04, LZ09, MN02, MZ05, MB03, MHT01, MC06, OFB08, PDC08, PSMB05, Qua04, RSKB03, RC02b, RK04, SAM06, Sch03, SBL05, SYC03, STH02, SE08, SDL07, SS07, TBG00, TCR02, TBGR04, VMA03, VC04, VMF03, WMK07, WM00, WM04, WM08, WCL05, WM01, YLL09, ZM03, vDSS04, LAS01].
methoxycarbonyl [KK09]. Methyl [CADW03, CCK01, DBM03, DMN05, HT05, RC04, WLX+05, WDZS07, WSM+08, WLL+03, WC08, ZLLS05].
methylacetamide [MMPK01]. methylacetylene [ZKZ+07]. methyamine
[LM08], methylation [EL07, HM08, SLC+09]. methylene [LFS+07].
methylenimine [dOMSL01]. methylenimmonium [dOMSL01]. methyl-
limazol [HT05]. methyloxaziridine [ZPL07]. methyloxirane
[ZPL07]. methyltransferase [WC08]. MF [DHW+08]. MF-3D-QSAR
[DHW+08]. Mg-porphin [ˇSBL05]. Mg [WZZ+09, AS06, LST08, ˇSBL05] +
WDS07, WSM+08, WLL+03, WC08, ZLLS05].
methylacetamide [MMPK01]. methylacetylene [ZKZ+07]. methy-
amine [LMB08], methylation [EL07, HM08, SLC+09]. methylene
[LFS+07]. methylenimine [dOMSL01]. methylenimmonium [dOMSL01].
methylimidazole [HT05]. methyloxaziridine [ZPL07]. methyloxirane
[ZPL07]. methyltransferase [WC08]. MF [DHW+08]. MF-3D-QSAR
[DHW+08]. Mg-porphin [ˇSBL05]. Mg [WZZ+09, AS06, LST08, ˇSBL05] +
WDS07, WSM+08, WLL+03, WC08, ZLLS05].
methylacetamide [MMPK01]. methylacetylene [ZKZ+07]. methy-
amine [LMB08], methylation [EL07, HM08, SLC+09]. methylene
[LFS+07]. methylenimine [dOMSL01]. methylenimmonium [dOMSL01].
methylimidazole [HT05]. methyloxaziridine [ZPL07]. methyloxirane
[ZPL07]. methyltransferase [WC08]. MF [DHW+08]. MF-3D-QSAR
[DHW+08]. Mg-porphin [ˇSBL05]. Mg [WZZ+09, AS06, LST08, ˇSBL05] +
Sie01, BA03, BA04a, BZP09, BM08, BSH07, CLP09, ČJPZS08, DJT08, DMM05, EDA04, ENM+04, GL04a, Gor01, HBM06, HSM06, HMMS09, HRZK03, HP04, Hin00, JM07b, JTR05, KCL06, KS01a, KJP+07, KVS+06, KPZK06, LEK07, LLL+08, LFR+04, MMLC05, MBM+00, MPF00, OFB08, SPGS08, SGS03, SYY+03, SPF+07, Sto05, TTB09, VBGL+00, XLC08, YKK09, ZBS03, ZMH+09, BBC+05. **modelling** [PSHP08]. **Models** [JB04, AS09, AHGK09, ACM+06, CCK01, CPUGD09, CRGN07, CA04, CA07a, CCT+03, DMM03, DLG00, DR07, DDVD09, EC06, FWH+07, FK07b, GS09, GV03, GS02, GDPCPU07, GDPP08, GS08, HMD05, HD06, HP01, HLT+05, HG08, HJCP01, JPF+00, KS02a, Kr03, LJKL08, Ls06, LS08b, MTC07, MTE04, MA05, MC06, OGH05, OYH05, PFJ+03, Pa05, QSS01, RD06, RSP03, RSER09, RS08, RR05, SBLK01, Sch00, SS+09, Srb02, SKK+07, SB01, SL06, VBS09, WB04a, WB04b, WB05, WZXY07, YCB00, YGLvG06, YJF06, YKK09, ZLJS03, ZCL09, ZGFL01, ZLDO9, ZWP08, TDH06]. **Modern** [PB02, FLK+07, Pra01]. **Modes** [Gra07, LSY02, MGLL03, OR05, Tor02]. **Modification** [HNL08, Vya01, YWH04, CM09, KFZ03]. **Modified** [LC06, NTH09, RC04, AVS09, CLA+00, KKY01, NA06, VVS07, WCs09]. **Modifying** [XLT07]. **Modular** [EA06]. **module** [HMD06]. **moduli** [LZZC09]. **MOF** [TAS07]. **MOF-5** [TAS07]. **Moffitt** [Kar01]. **moiety** [LBG08]. **Moldyn** [RMHK03]. **Molecular** [AS09, BBG+04, BG07, BDW00, CLC09, CLFA07, CCK01, DJT08, EMP07, FEVM01, FPN+05, GJK00, HLB09, Ish03, JTR05, KSB09, KAS+07, KLB03, KIM+09, LLA01a, LLAA01b, LLAA01c, LLA01d, LLA03, LSWB00, MLA00, Maz01, MO9, MS00, MST+08, NBJ04, Pin01, RMP01, RRZA08, SDD+08, SDM02, VSW+03, WEE01, YSA+03, YGLvG06, YK09, ZCS03, ZWS+09, AM09, AR10, AS06, AG00, ALB09, AD00, AGMPRG+08, ATMK03, AM06b, AB09, AGO+02, AP05, AS00, BG03, BP00, BR07, BA08, BB05, BWE05, BRDC02, BWZ08, BVW04, BT00, BS0B05, BME05, BS01, BPC07, CM08, CC07, CDS09, CCL06, COS01, CW02, CIB05, CDD+02, CKF08, CCSJ00, CGBF05, CF06, CF04, CPC+00, CR02, CCP07, CMD+04, CSU05, CBH+03, DvG00, DB07, DPT03, DFH05, DFG09, DPDG05]. **molecular** [DSS03, DMC05, DLHC06, DK01, DWC+03, ESM06, EK02a, EKB02b, F09, FHR07, FG02, FOK+04, FKL+06, FI+07, FBDG06, FL07, FAB+00, FKZ09, FEV+09, FKRE08, FNP+06, FRLN09, FKU+05, FK+06, GL04a, GLP08, GKR08, GCCV00, GLMV09, GFS05, GL08, GRD01, Gly06, GS02, GS03, Gon07, GSTD09, GCD+08, GS04, GKT04, GPK05, Ham07, HB09, HHHG08, HYT05, HGMB04, HH04, HEL09, HM08, HLS07, HSW01, HN02, HP04, Hin00, HIA03, HTK08, HK08, HW03, HTN03, IKN08, ITS05, IC08, Ish04, IJ09, IKYM09, JS07a, JMD+02, JP09, JG05, JGF04, JHP05, JPRSM+05, KMH02, KFZ03, KGG+09, KM00, KCL06, KEB04, KKC05, KSY+00, KAK+09, KCK+08, KBL08, Kn00, KZRO03, Kol04, KIF07, KvGH01, KH06, KC01b, Kr09a, KPR04, Kri08, Kri09b, Kr03, KKS04]. **molecular**
Monosilicon-substituted [YDWS06], monosubstituted [COMR’04, Lee09]. monoxide [GGP09, HT05, YQHQ09]. Monte [NCO’05, SCS07, AGSFAL05, AGSFA’05, BR03, BHG03, Der00, FCK’08, FKFG08, GHH07, HMD06, IM06, IKYM09, KLS02, KM07, KKKC05, LML+00, LZA02, LRWG03, MH09, Nak02, NA06, OM04, SKGS00, SB108, SM08b, SWR06, TS05, XKG+05, ZCS04]. Monte-Carlo [KLS02]. montmorillonite [DJT08]. MoO [LZZC09]. MOPED [SRCD03]. MORPHY [MP03b]. Morse [SDCG02]. Mössbauer [HLLN06]. most [KAS+07]. motif [HHW+03, LLL07]. Motifs [HWTL03, WHH+06]. motion [BRDC02, CCSJ00, LPK07]. motions [HSWN01, KS05b, LV08]. Mott [RDM+08]. MOVB [MG00]. move [SM08b]. moving [CvG08]. MP2 [BP02, EA08, FJP07, GCCVB00, IPN06, IPN07, JPF+00, ME06, PFJ+03, PMC+08, SAM06, WD04]. MP2/cc [WD04]. MP2/cc-pVTZ//MP2/6-31G** [WD04]. MpProp [SKK+07]. MPSim [CWV+05]. MRCI [SZW+05]. MSINDO [BGJo1b, JGH00, JW00, NB Jo04, SBG09b]. MST [COL01, CSB’03, FBLO08, MBH+02]. MST-based [MBH+02]. Mulliken [GHBB04]. multi [ABWT09, SL09]. multi-region [ABWT09]. multi/heavy [SL09]. multiatom [SSB+03]. Multibaric [OO06]. multibody [CPC+00]. Multicanonical [HHHS01, SKGS00, YC¸BM00, KH01, YAC¸02]. multicenter [DBS08, MS01]. multicentered [DWN01, HT03, WBSR03]. multicomponent [ST04]. multiconfiguration [NUH02]. multiconfigurational [GD06, PJPdPRMI07]. multicore [KHF+09]. Multicut [LSHR04]. Multicut-HDMR [LSHR04]. Multidimensional [AL01, ARLO1, Chn07, HP05, FC00, PFC03, RNG03]. Multidimensionality [FVB08]. multiensemble [HKMS01]. multieponential [GC03]. multifarious [Sim07]. multifield [BRDC02]. multigrid [BB05]. Multisotopic [Gar01]. multilayer [LJZ+07, SJJ+04]. multilayered [MR04]. multilevel [BHWW00, HBW01, JNV08]. multiobjective [CMBC08]. Multiple [CLF+09, CLZX09, DHW+08, JW06, SK09, STH02, BYQS03, CV09, GoL09, KM00, KH06, LJJ+06, MST+08, PAT+09, STCJ08, XOW+00, PYCD03]. multiplications [SSB+03]. multiply [HT03]. multipoint [WS05b]. multipolar [DWN01]. multipole [Ami00, ATMK03, BH03, CRG01, GY08, KM00, KLM+09, Mar03, RP07c, SF07, SG01, SvDS01, TFRZG01, VC04, WL09a, WBSR03, YOB+08, ZFL+05]. multipole-based [WL09a]. multipoles [KS01a, SKK+07]. multipopulation [HHJ03]. 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]. mutagenesis [MFR07]. mutant [DLRZ09]. mutants [GDPCPU07, MRS+07]. mutase [HHBH00]. mutations [HFS+07]. mutual [HTKG08]. mutual-information [HTKG08]. MXO [HT05].
myoglobin [AZS+04]. myosin [HSWN01].

N [GR07, JD09, KYFW07, KSN01, LS08a, LWW+06, Lu09, Mck07a, Mck07b, OS08, Sin07, TK08, WDXX06, WD08, WJX+08, XWXC08, YHD+06, ZY01, ZXY03, RMHK03, ZJ04, ZO4, CPC+00, DRAS05, FJ08, FH01, HD0+02, KKH+07, KBL08, Lu09, LKA01, Mck08, Mck07b, PFC03, RFSS06, SN00, SRE08, WLL01, Wii01b, WC08, WJX+08, ZW09, ZX09]. N' [WJX+08]. N-dimethyl [WJX+08]. N-dimethylhydrazone [Lu09]. N-formyl-serinamide [PFC03]. NaCl [PK04]. NAMD [PBW+05]. Nano [Est07]. nanoalloy [LJS05]. nanocomposite [DJT08]. nanomaterials [GJL+08]. nanomedicine [PSCD+09]. nanoneedles [PSCD+09]. nanoparticles [CGG06, KEM08, ZWC+09]. nanotubes [BG07, ZZvRSC08]. nanowire [KK08c]. naphthalene [CDPL09, HRG07, WL09b]. naphthalene-like [WL09b]. naphthoic [CMLS05]. naphthylisoquinoline [BMRF01]. native [BS01, yCkHM08, DBI02, MMMY07, ZCL09, ZS04]. native-like [DBI02]. Nature [CQ04, SK08, Ang09, KSK00, PYS05]. Nb [WD08]. nbo [Kar01, BPC01]. NCH [KRLD09]. NCN [LD05a]. NDDO [CSB+03, FA01a]. NDDO-based [CSB+03]. near [BVW04, PABK03, YL09, ZS04]. near-minimal-volume [BVW04]. near-native [ZS04]. near-neighbor [PABK03]. near-solute [YL09]. Nearest [HDF+07, HTKG08]. Nearest-neighbor [HDF+07, HTKG08]. NEB [GF08]. needle [BS01]. Negative [BLO+02]. Neglect [Lai07]. neglected [WCF04]. neighbor [HDF+07, HTKG08, PABK03]. neighbors [RP07d]. nematogenic [CLP09]. neopentyl [YTY07]. Nernst [DAK08]. net [BED02]. Network [KYL03, AG03, CLC03, Go09, GDPP08, GAS04, HSMMO6, KEB04, LSY02, MLGL06, NINAT+07, SJJ+04, SPT+03, UHNN09, WX09, LMH+09]. network-based [GDPP08, GAS04]. networks [BMRDB01, BSH07, FCK+08, KV+07, LJZ+07, PS09a, RLA01, TCSM03, VGDS08, dVB01]. networks-based [PS09a]. Neural [GAS04, AG03, CLC03, Go09, HSMMO6, KEB04, LJZ+07, NINAT+07, PS09a, RLA01, SJJ+04, TCSM03, WX09, dVB01]. neuronal [SBG+09a]. Neutral [DWS+09, ASS+02, Bac09, CYM02, DLR+08, EBDDM00, FCP+05, MT03, OSA06, PGG06, ROG00, VM02, Wn09]. neutrals [LXSS02]. neutron [BACJCT01, RMHK03]. nevirapine [AJNG01]. new-generation [YFJ+06]. Newly [CRS05]. News [An04b, BACJCT01, DV01, GLY06, JVVK09]. Newton [Har04, Qua07]. NF [FJ08]. NH [DMNO5, LF02, DOMSL01, DRAS04, ITS05, JPF+00, KTO8, KSTC01, LDMR01, MR02, Mck07b, PC00, SEKS09, dOMSL01]. NHC [ZWL+08]. NHNN [LWY+09]. Ni [Bac09, KGL07, PNM06]. NiAt [ZL07]. niches [TP01a]. nickel [Bac09, Gk09, LMIF06, YQHH09]. nicotine [VB09]. nicotinic [GCD+08, SBG+09a]. NiH [ZL07]. NiO [SBG09b]. niobium
NiSOD [PMM06]. nitrate [CGB+09]. nitrenium [FG03]. nitric [JDWS06, LPP06]. nitride [UNM+01]. nitrides [LX07]. nitrido [Bac05]. nitrites [POJ01]. nitro [MA05, POJ01, UTH+03]. nitroethane [GWM08]. nitrogen [BDWS06, LPP06]. gThDjL+01. WC08, XWL+09, ZLLS04a, ZLLS05, ZWY+09, ZMH+09]. nitrogen-containing [LMM09]. nitrogen-pivot [ZWY+09]. nitrogen-vacancy [ZMH+09]. nitrogenase [Ano06a, Mck07b, ST06]. nitroguanine [JM07a]. nitromethane [LZJ03]. nitrones [MGG06]. nitroxyl [LPP06, VCM01]. NLOPredict [MMP+07]. NMR [AGI+07, BPC01, BRDC02, CADW03, CMD+04, CMA+08, FO04, HP05, KIt+03, KBLP09, MC06, PC00, PFC03, PF06, RI07, RSER09, ZPL07]. NO [LDT+02b, PGNG03, PGRRNG03, ZLLS04b, ZLLS06b, IS03, FJ08, GBH+09, LDT+02a, MR02, PGNG03, RAGL09a, XDS06a, ZLLS06a]. Nobelium [HdMdS05]. noble [SRB06]. nodal [HYT05]. nodes [Kau07]. NOE [AGI+07, PF06]. non [GZ07, Gon07, SVT09]. non-bonded [Gon07]. non-Dyson [SVT09]. non-IPR [GZ07]. Nonadditive [Don08, PMB04, ZWP08]. nonbonded [ASDP+06, ATMK03, DK01, GWM+00, KH06, PABK03, SF05]. nonbonding [IB04, ZTS09]. noncentrosymmetric [GBJ03]. Noncollinear [Van02b]. Noncovalent [Won09, JˇCHS07, SP05, SMV+09, TH02]. noncovalently [PHFC04]. nonelectrostatic [KF02b]. Nonempirical [KSK00]. nonequilibrium [FZL+06, GG09, KK08c, LF04, LFZS04, OD09, YZ04, ZFL+05]. nonhybrid [DF04]. nonisomorphic [CRGN07]. Nonlinear [RLA01, BF04, BF07, Hart04, HLSH05, MMP+07, WCL05]. nonlinearity [LPK07]. nonmetallic [ALC08]. nonnative [yCKhYM08]. nonnucleoside [AJNG01]. nonorthogonal [SMZ05]. nonparametric [HDF+07]. nonplanar [Din00]. nonplanarity [RKH03]. nonpolar [GZL02]. nonrelativistic [WL02]. Nonspecific [LPB03, RGG08]. Nonuniform [SHSF05, Bie04a]. norbornadiene [WXY08]. norm [RRS09]. normal [EBAN07, KSU03, OR05]. nose [BBG+04, QNF09]. Note [An04b, An04a, FBS09]. Notes [CDGS09, CDS09]. Novel [IKN08, QCK01, QCK02, WZXY07, ZPL07, ZXY08]. 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, SBI08]. nucleophilic [BSB05, SS07]. nucleoside [Wil01b]. nucleosides [SA07]. nucleosome [VT+08]. nucleotide [Mak08, MSF+08]. nucleotides [WX08]. nucleus [FVB08, HdmS05, Hsd06, HD06, IKN08].
NUCS [SHSF05]. nudged [AJ03]. number [CD09, HX08, KZ06, KZw+05, KH06, TG0+00, WWL+09]. numbered [GYCZ04]. numbers [GDvC+07]. Numerical [DLW06, LX07, MO01, QN09, TO08, WL04, VW06, DB07, ESP04, FMA0, IO08, WL00, YK08, WG02]. Numerov [BiE04a, BiE04b]. Numerov-type [BiE04a].

O [BL00, GCCVB00, GPSP06, HYR06, ITS06, mJZ08, KGL07, LZZC09, LM09, Ma501a, Ma501b, NA06, Owe05, PGNG03, PGR03, UCT+03, WX08, YH+08, ZJ07, ZY01, ZL04, ZL+08, ZY03, Ba09, C0809, DR05, Dib05, HM08, HD0+02, IS03, LC07, LW04a, LS05b, MGL03, NY06, NH06, RA09, RF06, SS02, SRE08, W01b, YTY07, ZK09]. O-methylation [HM08]. O3LYP [BP03]. OB [NA06]. object [CR07, FL08, MVL+05]. object-oriented [CR07, MVL+05]. objective [WG02]. objectives [STCJ08]. objects [RSN+02]. observables [MG06]. observations [FWH+07]. observed [VB09]. obtain [BVW04]. obtained [HF03, VC04, WM03, WMW04, W08+06]. obtaining [Ba04, YGZ05, SK09]. occupied [HH08]. occurring [CJW+09]. OCF [UTM+02, UTU+04]. OCHF [YLW+08]. OCl [HLLS05]. OCLO [WLZ+07]. OCO [VM07]. OCS [VS02, ZGXX06]. octahedral [OSA06]. octan [BE07]. octan-1-yloxy [BE07]. octanol [COL01, CSB+03, Go09, T04]. octanol/water [CSB+03, T04]. octet [GR07]. Odd [CC07, GY04]. odd-numbered [GYCZ04]. off [HP01, LJK08, XLT07]. off-lattice [HP01, LJK08]. off-plane [XLT07]. OH [Dib05, G08, HT03, 1v06, LW04a, Ma501b, W07a, CU01, CUSS03, GAIM01, GCCVB00, GGL05, HT03, KZ09, KL09, LC07, LW0+09, Ma501a, MGL03, Mu05, RA09, RA09b, S09, UCT+03, W04, W07b, WY09, YL08, Y09, ZZL+08]. OH-initiated [RA09]. OH-rotamer [KL09]. OH-stretch [KL03]. OH/Ci [YLW+08]. OHO [Wi01a]. OHS [JP09]. olefin [PHG07, YXC+07]. olefins [AVB00]. oligomeric [EL07]. oligomers [BS07, CS01, Der09, LF07, S02, WCL05, ZOJ+06]. oligopeptides [MGJAC00]. Oligovalent [KS02a]. OLYP [BP03]. on-the-fly [KMA+07]. On-the-path [CY09, CY13]. One [CR09a, BG03, Ba07, Bi604a, GKR08, KFD06, Kri09a, Lai07, LB05, ZS0+02]. one- [Lai07]. one-dimensional [BiE04a]. One-electron [CR09a, BG03, Ba07, GKR08, KFD06, Kri09a, LB05]. ONIOM [BG0+09, MA08, MC06, VM+03, XKL03]. ONIOM-molecular [MA08]. ONO [FJ08]. onto [NK06]. OOPSE [MVL+05]. open [CSV+07, FS02, PRS+03, LA01]. Open-chain [LA01]. open-shell [FS02]. open-source [CSV+07]. opening [SRE08]. OPEP [AC+03]. operating [DFW05]. operation [PCA+08, SYC08]. operators [KM+02, Qua04]. OPFMM [CRG01]. OPLS
OPLS-AA [KB02, KOML08, KDSV02, MT03, POJ01, PB05, XLT07]. OPLS-AA/L [KOML08]. OPO [KZY09].

Oppenheimer [ZWZ09]. Opposite [JSHG07]. Opsin [RG02]. Optical [Bou01, CZFH07, CTF08, Hua09a, KSB09, LC09, LFR07, MA09, SN06, TDK07, WCL05, YFR05, Zer08, ZX08]. Optics [MMP07]. Optimal [GFS05, ACD03, BSP06b, Blo04, CRG01, DDVD09, SPT07, TTBM09].

Optimization [Ano06c, GL04b, GKH05, IK00, WCS09, WM12, AJ03, AM06a, BP00, BdPRMAI00, BM00, Bud07, BLM08, CS02, CZB07, COS01, CYM02, CLH07, CY09, CY13, CHM05, CMB08, DMN03, DV02, FM00, FRLN09, GHMP03, HHH00, HLTLP09, KKG09, KBA04, KHF09, KK01a, LJKL08, LJ04, LS05a, LJS05, MKT04, MM03, MM00, MW00, MGJAARC00, Pen06, PU09, Pu05, RK04, SSC04, SYC08, SWM04, SSMW09, SE08, SBH02, STC08, VMP+03, WS05a, WS02a, WPS02, XZZ04, YL06, YCS07, ZBS03, ZZ08, vLBBR12, WZW06].

Optimized [KM07, VB03, VK06, BSDM04, FKFG08, LJZ07, MV06, MY08b, MY08a, WTKM06, WN03].

Optimizer [KG02], optimizing [QSS01, SRC03]. Orbit [Duk01, CR08, CR09a, DXW08, KRM02, KTM02, LB08, LXS08]. Orbital [KIM09, Pen06, WM12, ALTB06, AB09, AS00, CFK08, FOK04, FKL06, FII07, FDU05, FM00, FRLN09, GHMP03, HHH00, HLTLP09, KKG09, KBA04, KHF09, KK01a, LJKL08, LJ04, LS05a, LJS05, MKT04, MM03, MM00, MW00, MGJAARC00, Pen06, PU09, Pu05, RK04, SSC04, SYC08, SWM04, SSMW09, SE08, SBH02, STC08, VMP+03, WS05a, WS02a, WPS02, XZZ04, YL06, YCS07, ZBS03, ZZ08, vLBBR12, WZW06].

orbital-based [CFK08]. Orbital-correlation [SRE08]. Orbital-orthogonality [Pen06].

organic [ATH03, BLY06, BT00, CCK01, DA01, EDJ04, EBD01, GO09, HELM09, HP04, JLF03, JVK09, JTR05, KLH04, LH02, LJZ07, LMRV09, PO03, PB04, SSJ04, SYY03, TAS07, Van07, WCK00, YGZ05].

organizing [BA08, ZA07]. Organocatalytic [WSM09]. Organocopper [YIN03]. Organocuprate [YIN03]. Organometallic [Gor01, SYY03, TD08, TTBM09]. Orientation [BL00, MLW08]. Oriented [CRH07, FL08, MVL05, RMHK03]. Origin [JS07b, GYM07, KMM07].

Orthogonal [BA07]. orthogonality [Pen06]. orthogonal [Lai07].

overdetermined [RI07]. overlap [LKW04, SGPS09]. Overview [Sch03, Mac04]. oxazolidones [OY01]. oxazoline [XKG05]. Oxidase [BS06, JKL08, WZY04]. Oxidases [PS03]. Oxidation.
Oxidative [DGD+05, LL00, PMM06]. oxide [BSJ01, CFS+08, CCCJ09, JDWS06, JT08, LPP06, PV07, RRS06, SBB02, ZCS04]. oxide/electrolyte [ZCS04]. oxidizes [ZSC05, ZLLS05]. oxidized [CNN07, CR02]. oxidoreductases [CFS+09]. oxidosqualene [SGS03]. o xo [CN05, WJX+08]. o xo-porphyrins [CN05]. oxocarbonium [LSWB00]. oxoguanine [FPN+05, JM07a, Pin03]. oxohydrocarbons [Wil01a]. oxoimidazoles [JKM08]. oxonols [BG00]. oxygen [GTC06, GWM+00, MML+06, SO09, WSC09, XPW09]. oxygen-adsorbed [XPW09]. oxyl [AZM03]. oxyl- [AZM03]. oxynitrides [WD08]. ozone [YLZ08].

P [BAL+01, Gog08, KZY09, LS08a, Lip00, OS08, QB05, WZZ+09, ZY01, MK02, CCP04, Mit01, RPNJ07, RFSS06, Tot04, KZY09]. P450 [Ast06, HBM06, LCC09, ZAT07]. P450-catalyzed [Ast06]. P450nor [LPP06]. P450s [OYH05]. p8 [BRDC02]. PAnhar [GBDP05]. package [AGSFA+05, BACJCT01, CSV+07, GSDT09, IM06, KSY+08, Kli01, KWK+00, MABB09, OTL08, PVdB00, RMHK03]. package-independent [OTL08]. packed [AT02]. Packing [MM03, CM09, CA07b]. Packmol [MABB09]. PAH [Don08]. Pair [FK07a, FS04, GR07, HZX04, KSTC01, LBT07, MLL06, MGCA07, Ni09, PC05, RC04, SC01, SYC03, Sim07, PC07]. pairing [DP04, HWTL03, PC05, PC07]. pairlist [HH04].

pairlist-construction [HH04]. pairs [BM08, CJDK09, FZL07, KKMM05, PABK03, ZZW09]. pairwise [Ano05b, CLZ+09, MTE04, Sha05, VP02, VZM+08]. Palermo [Van08]. palladium [WCW08, WCH09]. palladium-catalyzed [WCW08, WCH09]. pancreatic [MBC08]. paper [JW12, WM12]. para [ASDP+06, KCO1a, ZK09]. para-didehydropyridine [KCO1a]. para-didehydropyridinium [KCO1a]. para-hydrogen [ZK09]. paradox [CDGS09]. Parallel [BWP07, DOSG06, MBWP03, TGGP+00, UIHN09, ASWG07, Ano05b, AGSFA+05, BP02, BW+09, CRG01, GBPD05, GS04, GKTS04, GPK05, HHJ03, HHHS01, IS07, IPN06, IPN07, KKC05, KOFF09, KVF+07, MVL+05, MGJAARC00, NK02, NG04, Sha05, SPT07, SY+02, TFZG01]. Parallelization [GJK+06, PVdB00, PV03, SZV+05, UKNS01, CCWH02, FOK+04, FCK+08, UKN04, VSK+04, VGGB00]. parallelized [TP01a, VK06]. parallelizing [SO07]. parameter [BLMS08, CRG01, CHMI05, HXL09, MO09, OVM04, SHK+05, FM00]. Parameterization [KB02, PNG08, SMM+08, TCT03, BGJ01b, FH01, JKL08, JGH00, LSWB00, MTE04, PB04, RKH03, TGLL07, VSW+03, WK01, JJB02, JVVK09]. parameterized [GB04]. parameters [AAP00, AMR04, Ano06c, ATBL04, BBG+04, BSDM04, BZL05, CYM02, DB06, DDDV09, FAR02, FSFK05, FRS05, HPL03, KFNH08, KOML08].

[AGSFA+05, BACJCT01, CSV+07, GSDT09, IM06, KSY+08, Kli01, KWK+00, MABB09, OTL08, PVdB00, RMHK03].
KVL+04, KC01b, MMMY07, MSR04, MRC03, MLL+08b, MC06, OYH05, OMN08, OBT09, PRKP05, RRCA08, SO09, SEKS09, SRCD03, SHD+08, SCF+09, TT05, TTB01a, VCM01, VIP+06, WZV+06, ZSK07.

**Parametrization** [PDS01, COL01, SBH02, WS05b]. parametrized [RSP03, TAS07], paraoxon [ZWS+09], parent [MD04, YLW+08]. Pareto [STCJ08]. Paris [HP04]. Parr [Kri09a]. Parrinello [JP09, Sch04]. part [AG1+07, CDS09, ESP04, GDPP08, LL01d, vDSSvA04, AGI+00, Rud05c, vEMK01, vE01]. Partial [Ike04, BSC, Gol09, KC01b]. partially [SVT09]. particle [Ano05b, CZB07, GY08, KM00, KSY+00, LJZ+07, Sha05, SJJ+04, SHH07, SZW+05]. particles [BCIB05, WWL+09]. particularly [BS06]. partition [CCK01, CSB+03, DP03, GLD08, Go09, RM07, TS05].

**partitioning** [ACD+03, DVP+02, DVRP+03, HSM06, RP07a, VC04, WHN03]. path [ABB01a, ABB01b, Bbo4, Bo01, CY09, GF08, GM08, JP09, Kli01, Qua01, UCT+03, VGB08, WHG+07, CY13]. paths [FG03].

**pathway** [LGB+09, WLL01]. pathways [AJ03, JW06, LK+04, MAF+07, Qua04, RAGL09a, RAGL09b]. Pattern [DGHR02, EK02a, EK02b, KEB04, AGMP+08, HD03, EK02a]. patterns [CGG06, Gor01]. Pauli [Ish03]. PB [GC04, WHF08].

**PBCAID** [QSS01]. **PBSA** [PB06]. PtTiO [ZXYF09]. PC [An01b, BMB01, HSMT04, OSH03]. PC-GA-ANN [HSMT04]. PCM [FKL+06, CR03]. PCs [HS07b]. Pd [DGD+05, GBBH09]. PDDG [RCJ02b, TBGR04]. PDDG/MNDO [RCJ02b, TBGR04]. PDDG/PM3 [RCJ02b, TBGR04]. PDE7 [DD08]. pea [PS03].

**PF06, WD04, MM05, OO08, SS+09**. 6-31G* [FSFK05, FKJ+01, NL08]. 6-31G** [WD04]. adsorbate [BW+02]. AM1 [FRS05]. AMBER [FSFK05]. As [KS05a]. carbazole [YFR05]. CASPT2 [WLZ+07]. CBS [Lu09]. cc-pVTZ [WD04]. CCl [ZL09]. C [YLF08]. closure [SW06]. continuum [LRI+02]. Cs [GLR02]. decomposition [ML00]. DFT [BRLS12, BRLS08]. dissimilarity [hYD+08]. DQ7 [KV+06]. electrolyte [ZCS04]. empirical [CYM02]. FE [AGK03].

**four-centers** [GYM07]. fractal [Fan07]. free [BG00]. Ge [LLX02]. GeH [LLX02]. heavy [SL09]. HLA-DQ8 [KVS+06]. implicit [LS04]. Kohn [RRS07]. L [KOML08]. metal [MSBS01]. MM [CGP05, MP00, AST06, CR09b, CG05, FRA02, FMSA06, FSFK05, GM08, GW+00, HBB00, HBM06, HR08, HRR05, HTN03, IV04, IvS06, ITS05, ITS06, KHF+09, KPR04, Kri08, Kri09b, MBM+00, MSH+06a, MG00, ML03, NGB03, RGO2, SBB+09a, SN06, SMM+08, SVV+08, TII01, TDMSD+08, VMF+03, WC08, WHG+07, WC08, YZ06, ZWZ09].

**MM4** [AD00]. Mn [BL01]. MNDO [RCJ02b, TBGR04]. molecular [CGP05, FÁ01a, MP00, TCR+02, VR07a, VR07b, XLZ08, ZAT07].

**MP2** [WD04, GKT04]. **MRCl** [KT02]. nonstable [GDPCP07]. NP [GZL02]. one-step [Oos09]. order [MO09]. particle [BYQ03]. PM3 [RCJ02b, TBGR04]. polarization [YL09]. poly [BS01]. QM
[AB09, HT03, SURG06]. QSAR [ZNLL07]. QSPR [TCSM03]. SA [GWS+02]. SAC [DHM+03]. SCI [TY03]. solvent [PMB04]. SSB [KVS+06]. statistical [ML00]. volume [Lab08]. water [CCK01, CSB+03, FBDG06, Tot04]. penicillin [MK02]. penicillin-binding [MK02]. penicillins [DSS03]. pentacarbonylmanganese [PYS05]. pentanes [BPC01]. PEPCAT [OML+00]. Peptide [Adc04, DHW+07, HJCP01, JPF+00, ONHN00, PFJ+03, BTP09, BWE05, BSP06a, CLWL09, CSJ01, CJW+09, CLA+00, CP09, DvG00, DWN01, GSB09, IGNH03, LHJ+06, LL01, MS03, MHT01, MST+08, OGH05, OKH+02, PHFC04, SDL07, Tot04, WFC04, Will1b, YZ06, YÇBM00, ZALMG03, ZCZ03, WHP02, KVS+06]. peptide/HLA [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, OM04, PCO+07b, PRKP05, PFC03, SJW09, WZW+06, YAÇ+02, ZW09, ZLD09, ZOJ+06, PCO+07a]. peptidomimetics [BAH+02]. percolation [Mei02]. perfluoro [FO04]. perfluorosulfonate [YSJ09]. perform [ME06, WCK00, WHG+07]. Performance [BM00, CUL04, CA04, DNN03, FOL+04, JM07b, KPKZ06, LLS03, RLD109, VBS09, ZM03, AM06a, BL05, BRV+07, BLMS08, CCWH02, DF04, DB06, DGI+08, FMPS08, KWK+00, KEM08, KS05c, LWH06, MA09, NYTH09, SF07, SCF+09, Sto05, SBH02, UKN04, WMK07, WL04, WSM+09, WM01, BP07]. Performances [CLP+05]. Periodic [PMC+08, AMI00, BVW04, DRMD03, FROD08, HH04, Kau07, KSS08, KAK+09, QSS01, SRB06, WM06, ZLD09]. peripheral [BGC+09]. periplasmic [CGB+09]. permeability [CRG+07]. permittivity [GPN01, PZS04]. permutation [SN00]. perovskite [WD08]. perovskite-type [WD08]. peroxa [BLO+02]. peroxidase [HBM06]. peroxidative [MR09]. peroxides [LLZ09]. peroxy [Dib05]. peroxyxynitrite [JM07a]. personal [May07]. perspective [KLQ+09, LMGO+09, PBH09]. perspectives [Fie02]. perturbation [CWY09, CPML08a, CG05, DRMD03, JSR+07, FII+07, Gri03, IN08, LK04, MRS+07, NUH02, Oos09, PMGL03, Pog06, QT+dG+08, RSE07, SWZS04, UTH+03, UKNS01, UKN04, Var09, WCFH02, WHN03, YH09]. perturbations [OV03]. perturbed [DOSG06, ZZW09]. pesticides [KEH+02]. PH [RD00, DR09, WDS06, MCM04]. pharmaceutical [KV00]. pharmacophore [BA08, JFG04, LFKL00, HHG+09]. pharmacophore-constrained [LFKL00]. phase [BAL+01, CPJ00, CPJ01, DR09, DGI+08, DWC+03, FBGD06, FM00, GLMV09, JJK+00, JHZ09, KSB+02, KT08, KFN08, KKH+07, LRI+02, Lee09, LB05, LLL03, MBF04, Mas01a, Mas01b, MM02, Mor02, POJ01, PV07, wQZsLyZ02, QNF09, RRS06, ROG00, SMGE08, SDcG01, SMK00, TK08, TDH06, UCT+03, UNM+01, WD04, XKKL03, XKG+05, YQQH09, ZALMG03, ZSK07]. phase-space [QNF09]. phases [ALC08, CLP09, LXS08, SK05, XBO8]. PhAST [HHG+09]. Phe [VKP+08]. Phe-Gly-Phe [VKP+08]. Phen [ZWS+02].
phenol [LL01]. phenols [HM08]. phenomena [KK08c, RSS09].
phenoxycarboxylic [XKKL03]. 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, MBL+00, PMM05, PHRR08]. phosphates [WOC+03].
phosphatidylcholine [CEP07]. phosphine [HT05, LL00, MGLD00].
phosphinine [FLOD07]. phosphinine-containing [FLOD07].
phosphininium [LTF+07]. phospho [RGP+07]. phosphodiesterase
[XLZ08]. phosphodiesterase-5 [XLZ08]. phosphohistidine [KVL+04].
phosphoimidazole [KVL+04]. phosphole [LFR07]. phospho-containing
[LFR07]. phospholipid [MCR08, RG08]. phosphomannose [RGP+07].
phosphonic [CJ+02]. phosphorus [LYK+04, LTF+07, Mit01].
phosphoryl [ZJM+07]. phosphorylation [HLT+05]. phosphotriesterase
[KZRO03, ZWS+09]. phosphotyrosyl [OO08]. photoabsorption
[CHRL09]. photoadsorption [ZMH+09]. photocatalysts [HZ90].
photochemical [Ama02b]. Photochemistry [GD06, SRE08].
photodetachment [LMCD09]. photodissociation
[JHPRSM+05, LXS08, WXX03]. photoelectron [VDM06]. photoemission
[RD+08]. photoexcited [SRE08]. photographic [Shn02].
photoionization [MY08b]. photoisomerization [GRO+03].
photosynthesis [An006b, CPM03]. photosynthetic [IN01, OON01].
photovoltaic [LMRFH+09]. phthalocyanine [CM09]. phthalocyanines
[LS02]. phycobilisomes [MAF+07]. phycocyanin [MAF+07]. phylogeny
[LXZ06, ZLY07]. physical [BR07, DHW+07, OFB08, OS08, SRE03].
physically [AE06]. physico [AGMPRG+08, Mat03, SB01].
physico-chemical [AGMPRG+08, Mat03]. physico-chemically [SB01].
physicochemical [CP08, CP09, FTLV01, KLM+04, KEM08]. physics
[DB12, SPL+02, WS07]. physics-based [DB12, SPL+02, WS07]. physico
[CDD+02]. physico-chemical [CDD+02]. piano [FKS+09]. piano-stool
[FKS+09]. picture [VBGL+00]. Piero [An006b]. pinacol [TTY07]. Piotr
[An006c]. pivot [ZYW+09]. pK [KKS04, ZCS04]. pKa [CFR06, OS06].
planar [CSB08, MMRV07, SRS07, SBG09b, Wam09]. Planck [DAK08].
plane [PSS+04, PSMB05, RLD109, VSK+04, XLT07]. plane-wave
[PSS+04, VSK+04]. plane-wave-based [RLD109]. planewave [YK08].
plaster [HP04]. Plastocyanin [SN06]. platform [Gan09]. platinum
[CSB08, SMM+08, Wam01]. plausible [CBS+03, SB01]. play [YJF06].
Playstation [LEV+09]. pleated [PGC05]. Plessset
[CPML08a, JRR+07, FRI+07, Gri03, IN08, JSHG07, Var09, WCFH02, YH09].
plot [KMH02]. plots [CLZ+09, SDL+09, SRE08]. PLP [PMM05]. plus
[AGMPRG+08, CG05, IN08]. PM3
[BM00, BSDM04, DC02, GM01, MSH+06b, TGLL07, TCT03].
PM3-compatible [BSDM04]. PM3/d [TGLL07]. PM5 [LKT04]. PMF
[Mue01]. pocket [BS08, MDA08, OYH09]. pocket-specific [BS08]. Point
point-charge [DWC+03, CRC+00, GGLR00, KGL07, KK08a, KFZ03, MGCA07, SRB02, TBSM09, WMS06, ZMH+09].

point [BMLV04, BAÂ,07, DLD+02, GMA04, HQ02, MP03b]. Poisson

points [BMLV04, BAÂ,07, DLD+02, GMA04, HQ02, MP03b].

Poisson [WB04a, WB05, ABWT09, BHW00, BH03, BF04, BF07, DLG00, DA08, FOL+04, GPN01, GCD+08, GGT08, Hê05, HBW00, HBW01, KWHH07, LDG02, NYTH09, PZS04, SAT04, Vas02, VZ+08, WB04b, ZGF01].

Polanyi [Nye07]. polar

polar [BAÂ,07, CYM02, CPML08a, EB04, FA01a, HLLN06, HSF08, PFC03, ZXYF09].

polar-neutral [CYM02].

polarizabilities [ZPL07]. polarizability [BP01, HK08a, HK08b, Mar03, Mor02, QCK01, QCK02, vGGB00].

Polarizable [CFK08, LLM09, Nak07, Ano06c, AGO+02, APG05, BCIB05, COL+06, DGI+08, FKL+06, GMW+00, GS04, GKT04, GPK05, HHP04, JZD+09, KSB+02, Kol04, LJ04, MPPK01, MBC08, OR05, PWHF+03, PWHF+04, Pom04, RGP+07, TFZRG01, WZW+06, YGLvG06, FCP+04b].

polarization [CGB03, CBH+03, EDW07, GGLR00, HK08a, HK08b, KFZ03, MR04, Maz08, RP02, SL09, WL09a]. Polarized [EdlVR+03, BSOB05, OBBS05].

poly [ASDP+06, CHA+07, CFD04, MGMM07b, Qau07, SBB02, ZALMG03].

poly-isothianaphthene [CFD04]. poly-para-phenylene [ASDP+06].

polyacenes [BPCD07]. polyacetylene [PM02]. polyacrylates [LZA02].

polyalcohols [KBLP09]. polyatomic [GGB07a, GGB07b, RLR94a].

polyatomic [GGB07a, GGB07b, RLR94a].

polyatomics [TP01b]. polyazidocubanes [JWB05].

polycoordinate [TGGP+00]. polycyclic [Bor03, CA07b, FVB08, MGMM07a, VS08].

polyenes [MW09]. Polystyrene [BCF+09]. polyketides [KB02].

Polymer [Mei02, BB+04, CZA03, DJT08, MM07, RRZ08, YJS09].

polymeric [Fau01, JCA+02]. polymerization [BG07, YCC+07]. polymers [CFD04, CA04, CA07a, DC02, Der09, Din00, DDBP09, HM01, LAEL01, OKE+02, SHH07, VIP+06, YYW07].

pseudopolymer [VVBV02].

polynomial [HDBD04]. polynuclear [HYR06, RRFC+03].

polyoxoanions [LFR+04]. polypeptide [Cri04].

polypeptides [CFM08a, IB04, KF02a, KF03, Nak02, VP09].

polyphosphate [MRC03].

polythiophene [CA07b]. POPC [JM07b].

Pople [Ano04a, EA08].

population [BLT03, BPCD07, Pul05]. population-based [Pul05].

populations [KBN02, porph, SBL05, SBL05]. porphyrins [NyHN06].

porphyrin-fullerene [CHRL09]. porphyrins [CN05, LS02, LWH06]. portable [SH07].

potassium [MCR08, HHS05]. potential [AMR04, AE06, ABC01a, ABC01b, BCNs07, BL05, Bo01, BB+09].
potential-derived [TBSM09]. potentials [ATM+07, CLC09, CPUGD09, CKW09, DBI02, FAB+00, FNP+06, GK09, GBJ03, HZX04, HHHS01, HZ06a, IKY09, KLM+04, KCK+08, KK01b, LI07, LHI09, LK03, LK04, LLW09, MCF05, MWE02, OR05, PML03, RLER04b, SMD2001, SPT07, VGDSU08, dSR08]. Powder [HWDB03, HHJ03, dGWH01]. powerful [PSDM00]. pp [Bic09, Lip00, Sta00]. PQS [BWM+09]. PR [AVS09, VVS07]. Practical [BMRDB01, PHR+05, Woo01, You11, Blo04, Sch03, SHSF05, SWZS04, WW03]. precalculated [ZMZ09]. preceding [CSD05]. Precise [Ami00, Ara04]. precision [CN03, GAdGM08]. precursors [CFD03, CFD04, DJT08]. predict [HL08, HZ06a, HZ06b, LL07, PB06, PJPdPRMI07, XSHC06, XLC08, YMT04]. Predicted [PDP02, IGL07, JARM02, KCL06, WS02b, ZCL09, ZGXX06]. Predicting [DR09, Der00, LKA01, ZLS03, AG03, CLXC02, CRG07, I008, KSM02, XWC09]. Prediction [AVS09, CLC03, CRK08, CJD09, DA01, ELK+09, FCW06, Go09, JIK09, KLH+04, KCK+08, KEH+02, KF03, KKS04, LCC09, NINAT+07, OFB08, Sch00, YCW+09, YYW07, ABÅ04, BED02, CLF+09, CLA+00, DB06, EK06, GP06, GAS04, HEP+02, HSM06, HG08, KZ09, KP05, KFN08, KE04, KK08b, KS08, KOFF09, KF02a, LEK07, LXW+09, LHP01, LLZL09, LW+09, MSF+08, MS04, NCO+05, NLL+09, PBJ+07, QHL09, RGG08, TKS+01, TLKT00, Tot04, VGDSU08, WFHP01, WHP02, WHF08, WX09, ZHH09, AGI+07, GCD+08, KVS+06, ZCS04]. predictions [BS01, BLB09, CP08, Ruv07, Van02a, ZLD09, vEM01, vE01]. predictor [Kol04]. preface [FA01b]. preferences [GSB09, KK09, LKJ+04]. preferred [DV02]. preliminary [KHM02, PMC+08]. Preprocessing [SHM04]. prerequisite [WHF08]. presence [LZA02, RAGL09b]. present [GR07]. Presentation [Rud05a]. preserving [QNF09]. pressure [Car02, MTB09]. pressures [TK08]. primary [HB09, JIK09, KBN02]. primitive [MV06]. principle [GJL+08, PRS04, ZDS+05]. principles [CS01, EBL+08, GD09, HZ04, Hua09b, KK08c, MLJ03, TK08, VP08, WLX+05, WZZ+09, WD08, ZXY09, ZHMW09]. prior [IK09]. priori [SPDS01]. prismatic [WL09b]. probabilistic [PJB+07]. probabilities [DP04]. probability [CFS03, DLW06, GCDL+05, Kni00, SK09, SCS07]. probe [CVR08, DMLI05, TH02, VSW+03]. Probing [PAT+09, WMKG07]. problem [ABB01a, ABB01b, Ano06a, Bof01, CCL06, HLTLP09, Qua01, ST06, TKH07, XOW+00]. problem-size [HLTLP09]. Problems [You11, ABWT09, Mat03, Vis02, Woo01]. Procacci [Ano06b]. procedure [AM09, BR03, CA07a, DLSVY00, GP06, KBT03, RS08, SSL02, SMM+08, YÇBM00, Zho06]. procedures [GT03, HSMT04]. process
[BZL05, LGB+09, ML00, Pac06]. processes
[Che01, GG09, KEM08, LDTS07]. processing [AGI+00, AGI+07, FEV+09].
processor [LEV+09, Yas08]. processors [SPF+07]. Producing [KBN02].
product [SFR07, YLW+08, YLWL09]. production [YQQH09]. products
[KYFW07, LZ05b]. PROFASI [IM06]. profile
[Ber03, CCB04, CCP04, GB02, ONHN00, Zho06]. profiles
[AHK02, CMBC08, OD09, YXC+07]. program
[AJ03, BBM+09, DRMD03, GCRD01, Gly06, GM04, IS07, Kli01,
KWK+00, MP03b, ME06, PFX01, PRJ02, QSS01, RMHK03, SFRS01,
SMZW05, TRS02, UHNN09, VB07, VKCK09, Zer08, BBC+05, BKS02].
programmable [Gan09]. programming [SPT07]. programs
[CBD+05, KSS08, MBP09, SH07]. projection
[FS00b, GKH05, GY06, Qua04, TKN+08]. projector
[BCC05, KS08, MBP09, SH07]. projector-augmented
[MOP+07]. prokaryotes [WHH+06]. prolapse
[HdMdS05, Hds06, HD06, TW03]. proline [BISB02, KK09]. promising
[JR01]. promolecular [Leh06]. promolecule [MS00]. promoted
[SBG09b]. promotion [KMM07]. propagator [SVM09]. propanal [RR05].
propanone [RR05]. propargyl [LMK01]. propellanes [PAS07]. propenal
[BS03]. properties
[AB00, AEE+03, ÁCD+03, Ara04, AZS+04, BG03, BZP09, BT00, BSOB05,
BACJCT01, CMM08, CDGS09, CDS09, CPDH08, CLC09, CRV08, CZFH07,
CDD+02, CHA+07, CRSB03, CTF08, CMA+08, DD08, DXW08, DWN01,
DVRP+03, DD00, DPM09, DS03, DHW+07, EM03a, EM03b, Fau01,
FTL01, GKR08, Hua09a, HJCP01, JPF+00, JWB05, JT08, KHY00,
KLH+04, KIP+07, KCL00, Kri09a, Kri09b, KG06, KPZK06, KQ01b,
LTQ+07, LWLS07, LC06, LPR07, LLLZ09, LMRFV+09, MV06, MM02,
MA09, NA06, HNN+07, NTO07, OBB005, OS08, PM04, PK04, PBF07,
PT01, PSS+04, POJ01, RAK+09, SB08, SKR+00, TZX01b, TZX01a,
Tor02, TDK07, UM03, VB09, VKCK09, VP08, WLX+05, WM06, WCL05,
YFR05, YZ01, XYYF09, ZWP08, ZQ08, ZSK07, ZMH+09].
properties-based [VB09]. property [BAÅ+07, JLF03, NLL+09, PSD+09].
propylene [QZL+04, RR05]. propynyl [Lee09]. prosthetic [ATBLS04].
protease
[BWE05, CLX02, DLG00, LZ05b, NLL+09, SPT+03, SVV+08, WHF08].
protease-inhibitor [SVV+08]. Protein
[LEK07, NCO+05, PB+07, ADM+06, AG00, AHGK09, BED02, BRDC02,
BMLV04, BS01, BSP06b, BS05, BSH07, BLMS08, CCC03, CLX02, CLC03,
CLWL09, CSL+09, CIB05, CLH+07, CRK08, CLF+09, CJK09, yCK08Y08,
CRH+07, CPUG09, CSRST04, DHH+03, DPPR05, DB06, DBI02, EBAN07,
FOL+04, FC06, FKM+06, FKM+07, GLD08, GH07, GLQ+04, GC04,
GDPC07, GdSM+07, GHMP03, GKK07, GZM09, GB04, HEP+02,
HFS+07, HP01, H01, HM06, HLTLP09, HLM05, HLT+05, HZ06a, HZ06b,
HZ08, HW09, HP05, ILK09, IM06, I03, JS07a, JMD+02, J09,
KFB05, KFNH08, KLS02, KCL06, KHF+09, KK01a, KIFK07, KH05, KF08,
protein [PSHP08, PMM05, PB02, PF06, PNG08, QLHL09, R108, RSR09, RL08, RS08, RK05, Ruw07, SM04, SLC+09, SW04, SW+05, SN06, SR09, SM09, STC+08, SL06, TLKT00, TGD05, VW00, VW04, VGO+07, VGDSU08, VGGMM05, VZM+08, WS05a, WS07, XZZ04, XSHC06, XLC08, XCW09, Yan04, YL06, YFS07, YPNE09, Yos02, ZP03, ZGFL01, ZS04, ZZ08, ZTS09, ZM06, dSR08, HLC09, PMB04, ZZTS09]. protein-DNA [PSHP08].
protein-environment [HFS+07].
protein-ligand [LXW+09, RK05].
protein-tyrosine [AG00].
Protein/solvent [PMB04].
proteinogenic [IKYM09].
Proteins [LMH+09, AG03, Ano06c, BBHD04, BCP03, BHH+09, CR02, DWNBO1, DNN03, DR07, DV02, DJ04, DJB02, DWC+03, ES00, ENM+04, FNP+06, GAS04, HB09, HH05, HHW+03, HL08, HJCP01, Ike04, IDMC09, IN01, KSB+02, KT02, KKS04, LR03a, LJJ06, LKA01, MK02, MSH+06a, MZL08, NAT07, OS06, OSHS03, OM04, PB04, PM04, PRJ02, RGZM09, 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, LL08, LMGO+09, LB05, MA05, PGG06, PCS04, SM06, WFHP01, WHP02, XKG+05, ZCS04, dSGCG00].
proton-coupled [CXZ+09].
protonated [CPDZH08, ZDS+05].
protonation [Bac05, CG05, DMM+03, HP05, KYFW07, WHF08, XZ05].
prototoporphyrinogen [WZY04].
prototype [Ang09, CS01, ASDP+06].
prototypes [SSS+09].
proximity [Agr03].
pruning [TCSM03].
pseudo [LL07, VDM06, XSHC06, XLC08].
pseudo-Jahn [VDM06].
pseudofolding [VGDSU08].
pseudoknots [DP03, DP04].
Pseudomonas [NYK+09].
Pseudopericyclic [LFS+07].
pseudopotential [FMAMVK06, MK03, VW03, vW06].
pseudopotentials [PSS+04, PSMB05, SMD02].
PSi3 [CSV+07].
psoraleen [NBTN04a, NBTN04b].
Pt [DM05, LWK08, LF02, RD00].
PtCl [LF02].
PtF [LF02].
PtH [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 [MD10].
pVDZ [Wib04].
pVTZ//MP2/6 [WD04].
PW [EBL+08].
PyFrag [VGB08].
pyrazine [LWX07].
pyrazole [DMM05].
pyrazoline [LLKC06].
pyrazolyl [HT05].
pyrene [HIA03].
pyridine [CHA+07, HT05].
pyridines [WRP+06].
pyridoxal [LDY+08, PMM05].
pyrimidine [LWX07, WXW08].
pyrimidinyl [WJX+08].
pyrolysis [KKH+07, KKKL03].
pyrope [ZWTP+08].
Pyruvate [ČJPZS08].
pyVib [Zer08].
Q [BS08, KWK+00, WHG+07].
Q-Chem [WHG+07, KWK+00].
Q-Dock [BS08].
QCISD [ZK+07].
QCT [DPM09].
QM
[CGBF05, MPF00, AGK03, AST06, AB09, CR09b, CG05, FAR02, FMSA06, FSFK05, GWMO8, GWM+00, HHBH00, HBM06, HNR08, HRR05, HT03, HTN03, IV04, IvSV06, ITS05, ITS06, KHFe09, KBLP09, KPR04, Kri08, Kri09b, LLL03, MMB+00, MK02, MSH+06a, MG00, MLJ03, NGTB03, RG02, SURG06, SBG+09a, SN06, SMM+08, SVV+08, THHN01, ThMsd+08, VFM+03, WCC08, WHG+07, WC08, ZWZ09]. QM/FE [AGK03]. QM/MM [CGBF05, MPF00, AST06, CR09b, CG05, FAR02, FMSA06, FSFK05, GWMO8, GWM+00, HHBH00, HBM06, HNR08, HRR05, HT03, IV04, IvSV06, ITS05, ITS06, KHFe09, KPR04, Kri08, Kri09b, LLL03, MMB+00, MK02, MSH+06a, MG00, MLJ03, NGTB03, RG02, SURG06, SBG+09a, SN06, SMM+08, SVV+08, THHN01, ThMsd+08, VFM+03, WCC08, WHG+07, WC08, ZWZ09]. QM/QM [AB09, HT03, SURG06]. QMCF [PHRR08]. Qmd [KMH02]. Qmd-plot [KMH02]. QMPFF3 [DGI+08]. QMQSAR [DMLI05]. QSAR [DHW+08, DHW+09, SGPS09, CGMPT+08, CMBC08, CRG07, DMLI05, DM05, GDPP08, HSMT04, HMMS09, LLL+08, LIZ+07, LSY02, MRS09, PS09a, SJ+04, TCSM03, VB07, VB09, VGDSU08, XYN+06]. QSAR-analysis [VB07]. Qsar/QSPR [TCSM03]. QSPR [CDGS09, CDS09, CDGS09, GS08, HM08, TTBM09, ZNLL07]. QSPR/ QSAR [ZNLL07]. QTAIM [GMIM07b, RKA+09]. quadratic [ABBC01a, ABBC01b, Bo01, HG08, Qua01, ZH09]. quadrature [CG06, DBS08, GC03]. quadrilaterals [GKK07]. quadrupolar [CMA+08]. quadrupole [HLLN06, HK08a, HK08b]. quality [BG03, CMJ08, EM03b, FKZ09, JBJ00, JJB02, SSS+09, TSSGS07]. quantifying [GT03]. Quantitative [Mit01, WZY04, YNZ+08, BAA07, CDGS09, CDS09, DHW+08, DHW+09, Gra07]. quantization [GLMV09]. Quantum [AVB00, BWM+09, BS06, DMN05, ECA06, ESM06, EDAJ04, FHR07, LB07, MBL+00, MA05, NKR+02, PM02, RM07, RON02, SC01, SS05, TLOG00, VHR07a, ZMH+09, AGM08+08, AGO+02, APG05, ATH+03, AGSF05, AGSF+05, BSJ01, BPC07, CL09, CDGS09, CZF07, Con02, CKW09, COL+06, DBS07, DBM03, DA01, DWM+03, EBD+01, FCK+08, FÁ01a, FAB+00, FKF08, FR06, FKO+05, GAIMVB01, GVATG03, Gog08, GBB07, GGLR00, GS04, HM08, HHP04, JJH01, JCH07, KSB+02, KFN08, KJVV08, KHY00, KZRO03, KLM+09, LHP01, MFBO4, MP03a, MGCA07, MKT04, MR09, MPB09, Mat03, MC06, MPF00, OYH05, OKH+02, PG04, PK07, PDS01, PV07, RP07b, RSE07, RGP+07, SF07, SH07, SS00, SA04, Sch00, SFRS01, SBB02, TCR+02, TT02, VHR+07b, Vis02, VKCK09, WS05a]. Quantum [WOC+03, XYN+06, XZZ04, XLZ08, ZCZ03, ZAT07, ZSK07, SB08, CGBF05, DS03, KBL08, PFB05, SCS07]. quantum-chemical [DA01, SFRS01, VKCK09, XYN+06]. Quantum-connectivity [EDAJ04]. Quantum-regions [SB08]. quartet [MSBS01]. quartet/metal [MSBS01]. quartets [MSBS01]. quartic [SAS05]. quartz [ZWPR+04]. 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]. QUILD [SB08]. quinolines [KS05c]. quinoprotein [JJH01].
quintet [GWL07].

R [Bo01, CPJ00, LZZC09, Lip00, Qua01, ZY01, LZZC09, ZPL07]. rack [OCP02]. Radical [GC03, ESP04, Kau07, Kni00]. Radial [XDS06a, AVB00, BL06, CUS00, CU01, CUS03, CXZ+09, GSB09, HIA03, JDWS06, KOML08, KKMM04, LC07, LMK01, NSB08, O004, gThDjL+01, WDWS06, WDS06, WDS07, WyLG+09, WLZ+07, WLL+03, XDS06b, YLWL09, ZLLS04a, ZLLS05, ZLLS06a, ZLZ+09, CXZ+09, QZZZ03].

radical-molecule [ZLLS06a]. radicals [BE07, Dib05, Lee09, WLLS04, WDZS07, WSC09, YLW+08, YLWL09, ZM03].
radii [OCB02, PML03]. radon [HD06]. Raf [GC04].

Ras [GC04]. reaction-diffusion [Bie04a]. reactions [AM07, BS03, CUS00, CFD03, Fie02, GAIMVB01, GMA04, GLH+08, GGB07a, GGB07b, HFHL06, HSWW00, JMI07a, mJlzLy07, mJlzLy+08, JH09, KYFW07, KIM+09, L00, LDC+07, MBL+00, NTH00, OY01, OY03, RNG03, Rao00a, RC04, RO01, Rud05b, Rud05c, Sch03, Sie01, SS07, TT08, TCR+02, UNM+01, VBGL+00, WLLS04, WLLS05, WDS06, WLL07a, WyLG+09, WDX+02, WLL+03].

Quasi-relativistic [VMA03, YH07]. Quasirelativistic [HWFN01].
quaternary [CW02, SO07]. quaternions [CSD04, CSD05, Kne05]. Quick [LMV07]. QUILD [SB08]. quinolines [KS05c]. quinoprotein [JJH01].
quintet [GWL07].

R [Bo01, CPJ00, LZZC09, Lip00, Qua01, ZY01, LZZC09, ZPL07]. rack [OCP02]. Radical [GC03, ESP04, Kau07, Kni00]. Radial [XDS06a, AVB00, BL06, CUS00, CU01, CUS03, CXZ+09, GSB09, HIA03, JDWS06, KOML08, KKMM04, LC07, LMK01, NSB08, O004, gThDjL+01, WDWS06, WDS06, WDS07, WyLG+09, WLZ+07, WLL+03, XDS06b, YLWL09, ZLLS04a, ZLLS05, ZLLS06a, ZLZ+09, CXZ+09, QZZZ03].

radical-molecule [ZLLS06a]. radicals [BE07, Dib05, Lee09, WLLS04, WDZS07, WSC09, YLW+08, YLWL09, ZM03].
radii [OCB02, PML03]. radon [HD06]. Raf [GC04].

Ras [GC04]. reaction-diffusion [Bie04a]. reactions [AM07, BS03, CUS00, CFD03, Fie02, GAIMVB01, GMA04, GLH+08, GGB07a, GGB07b, HFHL06, HSWW00, JMI07a, mJlzLy07, mJlzLy+08, JH09, KYFW07, KIM+09, L00, LDC+07, MBL+00, NTH00, OY01, OY03, RNG03, Rao00a, RC04, RO01, Rud05b, Rud05c, Sch03, Sie01, SS07, TT08, TCR+02, UNM+01, VBGL+00, WLLS04, WLLS05, WDS06, WLL07a, WyLG+09, WDX+02, WLL+03].
XLL^+02, XDS06b, YT04, YLW^+08, YLWL09, ZLLS04b, ZKZ^+07. Reactive [LLM08, Hir08, MMY07]. reactivities [HTSR04, YIN03]. reactivity [Ano06a, BM08, Bor03, BL00, CN05, FZL07, GTC06, MTB09, ST06, Tie09, TSSSG08]. reagent [DHW^+07]. Real [Woo01, You11, PBF07, PBF09, Sch04, THHN01]. Real-World [You11]. rearrangement [NSB08, PA05, ZGZX07]. rearrangements [LLKC06, YTY07]. Reassociation [DWNB01]. recently [RG08]. RECEPT [KC01b]. receptor [DLRZ09, FKV^+05, FKM^+06, FKM^+07, GCD^+08, HMK02, KBK^+01, MHL^+09, SBG^+09a, TFN04, TJE03, WS02b, XWC09]. receptors [CW02, FTLV01, NHH05, YKK09]. ReCO [HT05]. Recognition [UNHYT06, AGI^+00, AGI^+07, AGMPRG^+08, BR07, CW02, DGHR02, EKBO2a, EKBO2b, GdSuM^+07, KEB04, MSF^+08, PSHP08]. Reconstructing [BBP09]. reconstruction [Adc04, GKK07, KLS02, RS08, TGD05, WG02]. recoverin [LGB^+09]. red [McD08, SRK^+00]. red- [McD08]. redesign [GLD08]. redistribution [ZY01]. RedMD [GSDT09]. redox [GA^+09]. Reduced [BR04, BSOB05, OBBS05, ABBC01a, ABBC01b, BMLV04, Bo01, CNN07, CP08, DL^+02, EI07, GSDT09, HP01, Qua01, RS08, WEE01]. Reduced-size [BSOB05, OBBS05]. Reducing [PRSM02, SSL02, SY09]. reductase [CFER04, CGB^+09, CBC^+08, DBS07, GGLR00, HLTLP09, LRWG03, MCK07b]. 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 [KZY09]. region [ABWT09, Ana02a, HHHB00, WEE01]. Regional [TKH03, NTH09]. regions [HYT05, SB08]. regioselectivity [AVB00]. Registering [GBL^+05]. regression [DLWV07, Go09, GS08, LCC09, SY09]. Rehybridization [AM07]. related [ALC08, ACLK03, CFD04, KC01a, LXY^+09, LW06, LCDA03, LCGA03, LCA03, ML00]. Relation [SM08a, DVRP^+03]. relationship [DHW^+08, DHW^+09, JPCA08, KKW^+01, WLX^+05, KKW^+02]. relationships [BAA07, CDGS09, CDS09, CPUGD09, JLHF03, PSCD^+09, WZY04]. Relative [SWV^+05, LBL09, CG05, MML^+06, MRS^+07, RSE07, ZOJ^+06]. Relativistic [FFH^+01, NYH02, NSO^+07, SNM^+06, SMD02, WTKM06, YH09, ASS^+02, BHI^+09, Dy02, GHLK^+02, GPSP06, HdmS05, Hds06, HD06, LF02, SH02, Van02b, VMA03, WL02, YH07]. relax [GFS05]. relaxation [BRDC02, HSO1]. 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
[Bof01, CPML08b, WM12, CSD05]. Representation [GPK05, BB08,
CKR08, CF06, JIK09, LW04b, LZX06, LW06, RLR+04, WEE01, hYDN+08].
representations [BMI04, LAR+03, LR06, RS08, SN00, YNW05].
representative [YLL+09, YXL+09]. reproduce [VBS09, WS05b].
reproducing [MFB04]. repulsion [COL+06, Kri09a]. repulsions
[HGMB04, PBF09]. replication [BDW00, CFC+08]. requirements [AM06b].
research [JLHF03, PGH+04]. residual [RI08]. residue
[MH09, NBTN04b, PMM06, NBTN04a]. residues
[CFS+09, DHW+07, HJCP01, JPF+00, OS06, UNHYT06, XLT07].
resolution [BS05, BS08, CDGS09, JSR+07, GL04a, HXLS09, Nee03, WMRW+01, WS02b].
resolution-of-the-identity [JSR+07]. resonance
[BM07, FLGW00, MAF+07, WZXY07]. resonances [LMB08, PF06]. RESP
[WCK00]. respect [QCK01, QCK02]. response [HG08, OFIK09, vGGB00].
Restrained [SRB02, WCK00]. restraint [LJ07, LHI09]. restraints
[BS08, HWTL03]. restricted [BdPRMA100]. restrictions [KSB09]. results
[CSD05, LKT04, PFJ+03]. Retardation [HP04]. retention [RC04].
reticularum [HLB09]. retinal [BL05, LFEdL06, MSH+06a]. Retrieval
[CVR08]. reuptake [FPG+06]. reveal [DLRZ09]. revealed [HW09]. reveals
[Pin01]. reverse [AJNG01, ML00]. Reversible [DvG00, Kol04, NHN06].
Review [Bic09, CvG08, Lip00, Sta00, Woo01]. Reviews [LB99, Sta00].
Revised [ATM+07, SBB02]. revisited [ASY01, CVVB04, PCS04].
Revisiting [GPS06, JPCA08, LN01]. Rg [ZXY03, ZXY03]. RGF [HQ02].
rhenium [SBH02]. RHF [EA08, JPF+00]. rhodamine [VSW+03].
rhodium [GLH+08, LL00]. rhodium-catalyzed [GLH+08].
Rhodopseudomonas [IN01, OON01]. rhodopsin [CEP07, YKK09].
rhodopsin- [YKK09]. ribonuclease [KSK00, WOC+03]. Ribonucleotide
[CFER04, HLLN06, PCS04, PFR04a, PFR04b, TMBM02]. ribose [SA07].
ribosomal [SB01]. ribozymes [MMMY07]. rich [CZ05, LKW08]. Rigid
[SM03, DPRRR05, Din00, ECA06, FS98, FS00a, Ike04, Lهر06, LV08, KP05].
Rigid-body [SM03, Ike04]. Ring
[ZSE08, BE09, CDPL09, DC02, DLSVY00, FJ08, RPNJ07, SRE08, ZW09].
ring-structured [DC02]. RISM [MH08b]. rival [DDVD09]. RM1
[FBLO08, RFSS06]. RMSD [Kne05, CSD04]. Ru [Wei08]. RNA
[AM06b, DW08, GdAcV+07, LhWX07, LCSZ09, LOL+08, MB00, Mak08,
RTG00, SB01, YNW05, ZTST09]. 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, CPFL02, Ruv07, SVV+08, ZSC05, BY06, CDS09,
CFER04, Kau07, TFZRG01, VBGL+00, YT04, YTY07, YJF06, PMM06].
Roles [ALC08, IN01, NYK+09]. roll [FS98, FS00a]. room [TD08].
Roothaan [TW03]. roots [BdPRMA00, Nil09]. Rotamer [HLTLP09, GHMP03, KBLP09, LFBSK07, SMG09]. Rotamers [LMH+09, SHM04]. rotation [CMLS05, COMR+04, DHF+05, DBM03, HFS03, HK08c, LHI09, LZO05a, MGLL03, OMNH08, PBF09]. Rotational [CSD05, BVW04, KBN02, TS05]. rotations [IR03].
rough [Fan07]. rough/fractal [Fan07]. roughness [PHJ+08]. routes [GGGLL05]. routine [Kli01]. routines [AT02]. row [AD00, BP03, BGJ01b, JGH00, LK03, LK04, RRP+01, YTH01]. Royal [LWW+06]. RS [LAR+03, EK06, ELK+09, KEH+02, LRWG03]. RS-HDMR [LRWG03].
S [BSB05, Bic09, Gog08, HKHN08, JJK+00, KYFW07, MGLL03, Mck07a, Mck07b, WWS07, ZJM+07, ZY01, XZ04, ZALMG03, DLD+02, HTN03, MVLG06, MG00, RC04, RFSS06, SN00, WDS06, YT04]. S-network [MVLG06]. s-tetrazine [XZ04]. SA [GC04, WHF08]. SAAP [IT03, IT03, IKYM09]. SAC [DHM+03, HFS+07, HKHN08]. SAC/SAC [DHM+03]. saddle [DLD+02, GMA04, HQ02]. SAFE [AVS09, VVS07]. Sakurai [TKN+08]. Sakurai-Sugiura [TKN+08]. salts [JHMB+09, KWK+01, KWK+02, JHMB+11]. Salvetti [IKN08]. Salvetti-type [IKN08]. SAM [WC08]. SAM-dependent [WC08].
Sammon [FKZ09]. sampled [IZA06]. Sampling [IZK04, BHG03, CN03, CIB05, CY09, CY13, CV09, CvG08, CEP07, DDVD09, FKZ09, GT03, HKMS01, IS03, JW06, KH01, KM07, LKW04, Mak08, MH08b, MST+08, Nak02, NA06, RNG03, Rap06, SD09, SMG09, TS05, YL06, ZA07]. sandwich [JD09, RPNN07]. sandwich-like [JD09]. sandwiched [MHS05]. sarcoplasmic [HLS09]. SARS [LZ05b]. SARS-CoV [LZ05b]. SASMIC [EA06]. Sason [Bi09]. Sb [LS08a, XB08, XK08]. Scalable [PBW+05, VSK+04, Ano05b, KKK05, Sha05, VGO+07]. scalar [GPSP06, KBLP09, MP03b]. scale [DMN03, JO02, KK01a, MH09, MHW04, MFP00, ME06, Nak02, NA06, RRS07, SSL02, TY02+04, WCF04, WS07]. scale-transformed [Nak02, NA06]. scaled [CN03, JSHG07]. scaling [AL01, AR01, Con02, FR06, GGLR00, GY06, KLM+09, LJM02, OS06, RS05, SSB+03, SFS05, SKDO08, SP05, TCR+02, ZW09, vGVB00, vDVGJ00]. scanning [HMK02, MFR07, SMGE08, ZM06]. scattering [BACJCT01, Est07, HSW01, RMI03, WKU01]. SCC [ECM+03].
SCC-DFTB [ECM+03]. SCF [JHPRSM+05, PFJ+03, PVdB00, SAM06, VZVG06]. SCH [ZZW+07]. scheme [Bac04, FOK+04, IS03, JCA+02, JVV09, LVM07, Maz08, MSH+06b, RKA+09, SN00, SHH07, WS05b]. schemes [Bac04, Bac05, Bac07, PRS04, SPDS01]. Schleyer [Lip00]. SCMP [FÁ01a]. SCMP-NDDO [FÁ01a]. ScO [LMCD09]. Scope [LFE06]. scoring
screened [DHW00, FZL06, KV00, KSM05, LFKL00, LZ05b, PRDS08, SHSF05, YOB+08].

screening [DHW+00, FZL+06, KV00, KSM05, LFKL00, LZ05b, PRDS08, SHSF05, YOB+08]. SCRF [CCT+03]. SCUD [LZ05a]. ScX [WWS07]. SD [WLLS05]. SDCI [BM07, PRSM02, PRSM03]. Se [HKHN08, JJK+00, WWS07]. search [AM90, BR90, BMTSC91, CSJ91, CA94, GLD94, HHG+99, HXLS99, HM90, IZA94, KK94a, LFKL00, MGJAARC00, NL98, OGH95, OM04, Pul05, RHL99, Sau98, SE98, WK98, ZZ98]. searches [CZB07, YXL+09]. Searching [SPT07, STC+08, CvG08, Nak02, OYH99, SCC04, SYC08, YCS07].

Second [BC06, FS04, MO01, AKG93, JSR+07, DOSG06, FO08, IN98, JSHG07, LK04, QTdG+08, QCK01, QCK02, Rud05a, Rud05b, Rud05c, YTH01, YH09]. second- [LK04, Rud05a, Rud05b, Rud05c, YTH01]. Second-order [FS04, JSR+07, IN98, JSHG07, QTdG+08, Rud05c, YH09]. secondary [CLC03, CLA+00, DW98, DP93, GdAcV+07, IGNH93, LhWX97, LCSZ99, LW96, LOL+08, LLL97, MHT01, WPH+07, YNW05]. Section [Ano01c, Ano04b]. sections [MY08a]. seedling [PS03]. segment [YS00]. segmented [CGSdST06]. segments [BTLP03, GAS94, KF92a, YMT04]. segregation [Sza08].
set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

setup [GGT08]. set-up [GGT08].

set [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].

set-up [GGT08]. sets
[BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS0+07, OBBS05, OVMV04, RLA01, RLER01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04].

setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b].
Simulations [VHRR07a, VP09, WL09a, WCF04, WZW06, XLZ08, YNZ08, YGLvG06, ZCS04, ZSC05, ZGFI01, ZWS09, ZWZ09, ZSK07]. simulator [JGVF05, KIM09, MS04, SO07]. simultaneous [DDV09]. Singh [JVVK09]. Single [OV03, BG07, CV09, HSF08, IT03, IKYM09, LFZS04, WTK06, XWL09, ZzvRSC08, Mak08]. single-family [WTK06]. Single-nucleotide [Mak08]. single-sphere [LFZS04]. Single-step [OV03]. single-walled [XWL09, ZzvRSC08]. singles [IN08, WKYU01, dSVa09]. singlet [BLO02, CZ05, CG08, FG03, LS08a, OSA06]. singlet-dioxygen [BLO02]. singly [HHWG08]. Singular [FPG06, TBSM09]. Sir [Ano04a]. Site [CJW09, LLL07, AG00, CFR06, CF04, CFC08, CF04, GC06, FM00, IME02, IO08, JARM02, KVGH01, Leh06, LZA02, Oo09, PO03, PBZ00, PDS01, RR09, RZWS07, SHH07, TY09, Van02a, WS02b, ZP03, ZOJ06, ZX09]. six [GJK00, NL07]. six-site [GJK00, NL07]. sixth [CGBP09]. sizable [CA07]. size [BSOB05, EL09, HLTLP09, KS02a, KH06, KS02b, OBBS05, OV03, YAÇ02]. sized [SHH07]. Slater [CVVB04, EdlVR03, GC02, KG09, RLER04a, VB03]. Slater-type [CVVB04, EdlVR03, GC02, KG09, VB03]. slave [FR06]. small [CN03, Che01, CG06, FM00, IME02, IO08, JARM02, KVGH01, Leh06, LZA02, Oo09, PO03, PBZ00, PDS01, RR09, RZWS07, SHH07, TY09, Van02a, WS02b, ZP03, ZOJ06, ZX09]. small- [SHH07]. smallest [SRS07]. SMART
SMART-based [TTBM09]. smooth [GP01, KSY+00, PZS04]. smooth-particle [KSY+00]. smooth-permittivity [PZS04]. smoothed [LV08]. smoothing [HHPO0, ILB03, WS02a]. snapshot [YNZ+08]. SnCl [RD00]. sodium [FL07, MHS05, YSJ09]. SODOCK [CLH+07]. Soft [CckHmY08, ASDP+06, TLKT00, TJE03, TGGP+00]. 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 [CckHmY08, ASDP+06, TLKT00, TJE03, TGGP+00].

software [Ano04b, BACJCT01, DvL01, Gly06, JVK09, KB+00, PZS04]. Solid [CFS+08, CCCJ09, CMA+08, EGSG00, Ish02, KCK+08, SK05]. Software [Ano04b, BACJCT01, DvL01, Gly06, JVK09, CHB+05, GBDP05, KBA+04, MMP+07, NSU+02, BLMS08]. Solar [Kso5c]. solid [CFS+08, CCCJ09, CMA+08, EGSG00, Ish02, KCK+08, SK05]. Solids [vDSSvA04, JB04]. Solvations [VDR00, TLKT00, TJE03, TGGP+00]. solute [BBG+04, EDAJ04, KEH+02, LLW+09]. solutes [BBG+04, EDAJ04, KEH+02, LLW+09]. solubilities [SHH07]. solubility [BBG+04, EDAJ04, KEH+02, LLW+09]. solute [BBG+04, EDAJ04, KEH+02, LLW+09]. solute [BBG+04, EDAJ04, KEH+02, LLW+09]. solute [BBG+04, EDAJ04, KEH+02, LLW+09]. solute [BBG+04, EDAJ04, KEH+02, LLW+09]. solution [ADWM07, BACJCT01, DvL01, Gly06, JVK09, KB+00, PZS04]. solution-phase [TDH06]. solutions [Blo04, CPJ01, Loe03, PK04, VP09, XZ04, XZ05, ZWP08, LR03b]. solvated [HTSR04, HRR05, KHY00, QSS01, RSP03, BSC+01]. Solvation [COL01, HHP04, WB04a, WB04b, WB05, WD04, BCl05, CR03]. solution [ABWT09, BHWO0, BP07, BISB02, CPJ00, CCK01, CRSB03, DA01, ELK+09, FHR07, FG02, GAMA04, HHJ03, HMWC03, HSWN01, HRR05, HBWO0, HBWO1, HDO+02, KPR04, Kri08, Kri09b, KBNO2, LRI+02, LXFS08, LMIF06, MB00, MH08b, PD02, PTC01, PHRR08, RNG03, RRZA08, SH09, SATO04, SBB02, TDH06, VHS02, VBS09, YH06]. solution-phase [TDH06]. solutions [Blo04, CPJ01, Loe03, PK04, VP09, XZ04, XZ05, ZWP08, LR03b]. solvated [HTSR04, HRR05, KHY00, QSS01, RSP03, BSC+01]. Solvation [COL01, HHP04, WB04a, WB04b, WB05, WD04, BCl05, CR03]. solution [ABWT09, BHWO0, BP07, BISB02, CPJ00, CCK01, CRSB03, DA01, ELK+09, FHR07, FG02, GAMA04, HHJ03, HMWC03, HSWN01, HRR05, HBWO0, HBWO1, HDO+02, KPR04, Kri08, Kri09b, KBNO2, LRI+02, LXFS08, LMIF06, MB00, MH08b, PD02, PTC01, PHRR08, RNG03, RRZA08, SH09, SATO04, SBB02, TDH06, VHS02, VBS09, YH06].
special [AKA09, Bie04a, RP07b]. specialized [Kofo05]. species [CFC+08, DR09, GLH+02, HBM06, KZY09, WG02, YIN03, LMGR05].

Specific [FAR02, LR03a, BS08, HL+05, Pin01, PRJ02, SFRS01, TGLL07, TST+08, UHN09, WCF04]. specificities [PB06]. specificity [CJW+09, DLRZ09, LLL07].

specify [Fau01]. spectra [Bac09, BACJCT01, CNN07, CG08, Gor01, HKHN08, JARM02, KˇSB09, KFD06, LDL+09, MLCD01, NRKH02, OBB05, OKE+02, ŠBL05, SN06, TDL06, WM01, YZX+04, ZGXX06, ZWTP+08, dGWH01]. Spectral [II02, CVR08, GdSuM+07, LFZS04, NINAT+07, NAT07, SMKM00, WG02, ZSK07].

spectrometric [KZW+05]. spectroscopic [Ano06a, FCW06, KCL00, ST06]. spectroscopy [ACM+06, RDM+08, VDM06, WMRW+01, ZPL07]. spectrum [EL09, LMCD09, MWL+08, MGLDS00, PRSMM03].

speeding [KVF+07]. speedup [BYQS03]. sphere [HdMdS05, Hs06, HD06, LFZS04, SFR07]. spherical [BCIB05, ZFL+05]. spheriphane [CS01]. SPICKER [ZS04]. Spin [Duk01, HYR06, KTM02, LXXF08, Van02b, ACM+06, BB08, BACJCT01, CR08, CR09a, DXW08, DPT03, DF04, JSHG07, KRM+02, KRLD09, KˇSB09, LB08, Mck07a, Mck07b, VCM01]. spin-crossover [KRLD09].

spin-label [VCM01]. Spin-orbit [TDH06, WM01, YXZ+04, ZGXX06, ZWTP+08, dGWH01]. Spins [JD09]. Spino [HELM09]. spiroquinoxalines [DD08]. splines [ALK04]. splitting [EA08]. split-valence [EA08]. splittings [HLLN06, SFRS01]. Spontaneous [Sz08]. square [CS08, LLZL09, Nil09]. square-planar [CSB08]. squares [CSD05, GoI09]. Sr [WD08, SCP08, XB08]. Sr-doped [SCP08]. Src [O08]. SrFeO [Hua09b]. SrZrO [SM06]. st2nmr [PRJ02]. stabilities [ACM+06, CTFC08, GYCZ04, STC+08, WDXS06]. Stability [JD09, Owe05, PHFC04, WSC09, CJS+03, CF06, DB07, HXD08, JS07b, JBGK08, OCP02, PGC05, QB05, XFF06, ZXYF09, ZOJ+06, ZM06].

Stabilization [EBDPM00, HYA02]. stabilized [HSF08]. stabilizing [GZ07]. Stable [HD0+02, GDPCPU07, KYYW07, KZY09, KAS+07, Ko04, LMO09, PP08a, PZS04, STC+08]. stable/nonstable [GDPCPU07]. stacked [RRCA08, SJ08]. stacking [CM09, DDBP09, HWT03, KKY01, WRP+06].

standard [ASDP+06, CG06, FBDG06, KOFF09, LFSB03a, LFSB03b, SSS+09, SL04]. standing [KDG+09]. staphyloloccal [JS07a]. Starting [VZVG06, BWT+02]. state [Ang09, BBI+09, CWY09, CFS+08, CHA+07, Chu07, CAG07, CMA+08, HM01, HNF07, HNF12, Hir08, HP05, IME02, JH09, KTO2, Kri09a, LMK01, LZ05a, LDL+09, NTH09, PO03, PSS+04, POJ01, Qua07, SPGS08, Sen06, SRE08, TH02, TST+08, TY03, TKN+08, WCF02, WHF08, ZHO8, ZOJ+06]. state-correlation [SRE08]. state-specific [TST+08]. states [Ang09, ABBC01b, Bo01, Bov01, CWY09, CNN07, DYM+03, DF04, EL07, FCW06, FDSA00, HFS+07, HYR06, HZ09, IR03, KUB07, LS08a, LWX07, LB08, MW09, MLCD01, NBTN04a, [Bie04a, Bie04b, RP07b].
NBTN04b, OSA06, OV03, PRSMV08, Qua01, SB108, SMKM00, VW00,
WLZ+07, XZ05, ZL05, ZL07, ZL09b, ZM03, dSVA+09, ABBC01a]. static
[FROD08, LDG02, Mar03, XWL+09]. stationary [SK09]. Statistical
[HFS03, PYEA03, DW08, EC06, Kob03, RK05, SJ08].
statistical-thermodynamic [RK05]. step [BYQS03, BCP03, DLW06,
KM00, KH06, MK02, Mck07b, OV03, Oos09, ZWZ09]. step/particle
[BYQS03]. stepwise [LLKC06, LFS+07, NSB08].
stepwise [BYQS03]. Stereodynamics [CMLS05]. Stereoelectronic
[SK09]. Statistical [HFSD03, PYEA03, DW08, EC06, Kob03, RK05, SBJ08].
statistical-thermodynamic [RK05].
surrogate [Mck07a]. Surrouding [KGL07, Yos02]. Survey [HS07a]. SuSi [CA04]. SVD [CSD05, Wg02]. SVM RM [YMT04]. Swarm [CZB07, LJZ +07, SJJ +04, CLH +07]. Switch [SF07]. Switching [GG09]. Symmetric [AT02]. Symmetrically [Lai07]. Symmetry [PDC +08, PCA +08, BB08, CAGR08, FCP +04b, LWX07, SZW +05, WLPF05, Ell07, PV03, PTC01]. Symmetry-adapted [FCP +04b]. Symmetry-driven [PV03]. Symmetry-generation [Ell07]. Symmetry-adapted [FCP +04b]. Symmetry-driven [PV03]. Symmetry-generation [Ell07]. Synergistic [GS08]. Synthesis [CAG08, PHR +05, WLL01]. Synthetic [NHH05, WG02]. 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, BGJ01a, BWI +02, CN03, CG06, CvG08, CCK01, CMGDAC +07, DXW08, DRMD03, Don08, DK01, EGSG00, Ell07, 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, RLD09, RS05, Rud05b, Rud05c, SRS07, SS00, SY +03, SVW +05, ST01, TH02, TT08, WWL +09, WN03, YCY03, YZ04, vdVGDJ00].
CF04, FMPS08, KTM02, SBI08, SM03]. Testing [CMaGL+04, BG03, PZS04, WWC+04, WWC+05]. tests [KSB+02, NGTB03]. tetraammonium [CW02]. tetraazanaphthalenes [CdML+08]. tetrachloride [DMN05]. tetracoordinate [MMRVH07, SRS07, Wan09]. tetracyanoethylene [LH02]. tetraazanaphthalenes-contained [KSB+02, NGTB03]. tetraammonium [CW02]. tetraazanaphthalenes [CdML+08]. tetrachloride [DMN05]. tetracoordinate [MMRVH07, SRS07, Wan09]. tetracyanoethylene [LH02]. tetracyanoethylene-contained [LH02]. tetrahydroxouranylate [IvSV06]. tetracycline [AS06, AS09]. tetrads [MHS05]. tetrahydroimidazo [SPGS08]. tetrahydroimidazo- [SPGS08]. tetrahydroxouranylate [IvSV06]. tetramer [RRCA08]. Tetraoxide [JW12, SLHW09]. Tetrazine [JW12, SLHW09, XZ04]. Tetrazino [JW12, SLHW09]. Tetrazine-Tetrazine-Tetraoxide [JW12, SLHW09]. tetrazole [dSVA+09]. TGSA [GRCD01, GCD04]. TGSA-Flex [GCD04]. Th [NSO+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, BMS03, CNN07, CFD03, CFD04, CG08, COMR+04, FJ08, FL07, FDSA00, GYCZ04, GLH+08, HLLS05, HSL+00, IGL07, IIK09, mJlZyL+08, JW12, KYFW07, KZY09, KSB+01, KS05c, LS08a, LH02, LWX07, LDY+08, LLW02, LDT+02a, LDT+02b, LYZ+08, LMRFH+09, MMLC05, MCK05, MBM+00, NBTN04b, OCP02, OKE+02, PFR04b, wQZsLyZ02, RTG00, RZWS07, SLL+04b, SFR07, ST06, TKS+01, TJM+03, gThDij+01, VS08, WLL01, WLLS05, WDS06, WDXS06, WDZS07, WLL+07b, WCL05, WXJ+08, XFX06, XKKL03, YTY07, YIN03, YFR05, YLW+08, YQQH09, YLWL09, YHD+06, ZLLS04b, ZLLS04a, ZLLS05, ZLLS06a, ZLLS06b, ZZW+07, ZZL+08, ZZL+09, ZZW09, ZXY03, ZL07, BGC+09, CN05, DLR+08, GXX09, Ham07, HRBKB03, HLMR06, Kan07, KKIMS04, LC07, LD05a, Lee09, LL01, LLKC06, LB08, MM02, MDI04, NTH00, NSB08, Nye07, OON01, PGRRRN03, PC00, PAS07]. theorems [RAGLL09a, RAGLL09b, RRS06, RP04, RLLR06, SLHW09, SMV+09, UNHYT06, WLZ+07, WSM+08, Wou00, XWX08, XYZ+04, ZL05, dRLMS00, Li01, NBST04a, RD00, UNM+01, ZPL07, ZLD09]. theoretically [WS02b]. theories [JHZ09]. Theory [BBC+05, SH08, WM12, ALT06, ASDP+06, ASY01, BC06, CWY09, CFD08, CR08, Cui07, CWK09, CPM08a, Cui08, CGSDST06, DPM09, JSR+07, EL07, EKB02a, FCW06, FZL07, FG02, FII+07, FLGW00, FS04, FLK+07, FZL+06, GM01, GRL03, GRI04, Ha08, HSM04, HSL07a, Hold05, ION07, IKN08, IN08, JCHS07, KSS08, KWK+01, KWK+02, KKL06a, KZW+05, Kut07, LMB08, LF04, LHZS04, LMGR05, LF02, LLZL09, LDL+09, Lu09, MGMM07a, Mat03, MW09, MA09, MH08b, ML00, NYH02, NUH02, NTH09, OFIK09, OKE+02, PFJ+03, PSF+08, PU09, PA05, QTgD+08, RB01, RDM+08, RZWS07, SH07, SH02, SZT08, SSM09, SSB07, SW06, TST+08, Tru07, TKN+08, TJK03, WR0+06, WB07, WZY04, WMRW+01, WW03,
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[CAGR08, DRAS04, DRAS05, FSS00, GDPCPU07, HM08, JHFL03, MP03a,
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[RSER09, FCP05, GdAcV07, Kle03, KF03, KBL08]. Topology-based
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[CMC08]. Topo [HT05]. TopMXO [HT05]. tracing [KL01].
tracking [HNR08]. training [AG03, LJZ07, SJJ04]. trajectories
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[BZL05, CSB08, HKHN08, KMM07]. trans- [BZL05]. transamination
[LDY08]. transcriptase [AJNG01]. transfer
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Transferability
[CSB03, TT05, FDM00, KS01a, OSHS03, RSP03, TFZR01]. Transferable
[WSBR03, HXL09]. transferase [SFR07]. transferred [GFS05]. transfers
[XK05]. Transform [BWP07, HLM05, ON07, QLHL09, TYN05].
transform-based [HLM05]. transformation [PVdJB00].
transformational [CN03]. transformations [WSM09]. transformed
[Nak02, NA06, vDSS04]. Transition
[FKRE08, LMG06, TH02, ABY08, ABBC01a, ABBC01b, Ano06a, Bac05,
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Dib05, EL07, GHH07, GM01, Hol05, JH09, KR02, LW07, LD05a, LH02,
LGB09, LW09, LK03, LK04, NR04, PYCD03, Qua01, Qua07, RRFC03,
SK09, SHT08, ST06, TKS01, WB07, WL09b, YTH01, ZALM03].
transition-metal [Ano06a, ST06]. transitions
[CZ05, FC06, JW06, OYK07, SMK00]. Translation [RLER05].
transmembrane [GAS04, YMT04]. transport
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[BCF09, BZL05, CLA00, CBH03, HC08, HHH00, IB04, JB04, KS05b,
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triangulation [BHH09]. triazines [ZX04]. triazolinones [WZY04].
tribenzo [GLRL02]. chloroacetaldehyde [CU01]. tricoordinated
[LTF07]. trigonal [JHMB09, JHMB11]. trimer [LZJ03, RRCA08].
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[LLK06]. triosephosphate [AGK03]. tripeptide [VZ08].
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 [XF06]. TTTO [JW12, SLHW09]. tubular [FL07]. Tuczek [Ano06a]. tumor [WCF04]. tumor-specific [WCF04]. Tuning [JHMB+[09, JHMB+[11]. tunneling [Christ07, MKT04, RWBH09, SFRS01]. TURBOMOLE [LLL03]. turns [HL08]. Two [PFB05, Yas08, AMR04, AHK02, BRS07, BE09, CVR08, CCK01, DHF+[05, FBDG06, FR06, GGP09, GYMN07, GGA00, HK08c, JJK+[00, KAS+[07, KT02, Lai07, LDC+[07, LW-[06, Sen06, St05, Van02a, Van02b, YFR05, dSR08]. two- [Lai07]. two-body [FBDG06]. two-center [BRS07, GGA00]. two-component [Van02b]. two-dimensional [CVR08]. Two-electron [PFB05, Yas08, FR06, GYM07, GGA00, Lai07]. two-electron/ four-centers [GYMN07]. two-state [KT02, Sen06]. type [Bie04a, CZX+[09, CJK09, CVVB04, EdlVR+[03, GC02, Gri06, HLC09, IKN08, KDG+[09, Leh06, MY08a, OON01, SDL+[09, TLOG00, VB03, WD08, YXC+[07]. types [BY06, GGP09, KS05b, MLL+[08b]. Typical [SMV+[09, MLL+[08b]. tyrosine [AG00, CLS+[09, LRI+[02, Li01, LL01, OO08]. U [Han01, CCCJ09, GHLK+[02, RLDI09]. ubiquinone [IN01]. ubiquitin [KIFK07]. UCSF [GH+[04]. UF [Han01]. UK [Lip00]. ulcerogenic [CMBC08]. ultra [ZHMW09]. ultra-incompressible [ZHWMW09]. Ultrafast [BR07]. ultrasoft [PSS+[04, PSMB05]. umbrella [RNG03]. unbiased [Pul05, SYC08]. uncertainty [SY09]. unconstrained [DMN03]. uncorrected [PSC+[01]. understand [DSB+[02]. Understanding [CAGR08, CDPL09, BRS07, ZZW09, CFER04, HP04]. Unicorns [FK07b]. Unified [GDPP08, CMGDAC+[07]. uniform [HdMD05, HSD06, HD06, Rap06]. Unimolecular [ML00, FS00b, KZY09, ZL04]. unique [KT02]. unit [VM07, Yas08]. unitary [KBT03]. units [CXZ+[09, FEV+[09, HP05, NK01, NL08, PC00, PFC03]. Universal [DHW+[00, HDM05]. Unorthodox [KBB09]. unphysical [OV03]. UNRES [HXL09, NCO+[05]. unrestricted [YH07]. unsaturated [BS03, KFD06, MTB09, Wan09, ZKZ+[07]. Unusual [XX08]. UO [IV04, IV506, RDM+[08]. Update [BKS02]. updated [Chun07]. Updates [An04b, BACJCT01, DL01, Gly06, JVVK09]. upon [OFIK09]. uracil [LMG0+[09, MSBS01, MHS05]. uracil-base [MHS05]. uronyl [IV04]. Urea [SK05, AS00, VVS07]. ureases [ESM06]. Use [BWI+02, DW08, Wou00, ALB09, JNV08, KLI01, MRC03, OCP02, PRK05, PRS04, RCJ02a, RSN+[02, Ru07, SH07, SV09, VGGMM05, YTH01, YZ04]. used [DV00, ESP04, HDMD05, HDSD06, HD06]. user [DPD05, JKI08]. uses [KBB09]. Using [CSD04, FSM09, HL08, Kne05, LL07, MO01, OSH03, QLHL09, SW06, XSS06, XLC08, XOW+[00, Ad04, AJ03, ABWT09, AM06b, AS00, BW07].


BMLV04, BVW04, BME05, BGC+09, Bud07, CLWL09, CN03, CSJ01, CLC09, CKR08, CLA+00, Chu07, CP08, CP09, CCP04, CPML08a, CGSDST06, DLD+02, DWNB01, DR09, DVP+02, DB06, DBI02, DMJV05, EKO+01, EKB02a, EM03b, FCW06, FMPS08, FBDG06, FAB+00, FEVM01, FR06, FSFK05, GMA04, GL04b, GDSuM+07, GSP06, GGLR00, Haf08, HWDB03, Han01, HSMT04, HMM06, HMM09, HG08, HHP04, I02, ISO7, IS03, IT03, IK00, JBGK08, JIK09, JVVK09, JTR05, JFG04, JSHG07, KRM+02, KKG+09, KM00, KLH+04, KK+08c, KOFF09, Kle02, Kle03, KBT03, KKS04, Lab08, LCKL05, LCC09, LZ05a, LLL+08, L2ZC09, LS05a, LZ05b, LSY02, LKW04, ML+08, MT03, MMLC05, MKT04. using [MV06, MBP09, MOP+07, MTE04, MRS09, MRS+07, NCO+05, NINAT+07, OFB08, OKE+02, PBM04, PS+09a, PAT+09, PPS+04, RIO7, RI08, RPM01, RG08, RON02, SDL+09, SPS08, SS+03, Sch00, SRC+03, SBG+09, SY09, SPT+07, SMV+09, TP01a, Tie09, TCS+03, UBD+04, VSW+03, Van02a, WL+07, WL00, WEE01, WG02, WOC+03, WCS09, XLT+07, YKO0, YYYY07, ZCS04, ZBS03, ZWP08, ZHH09, vdVGD+00, PRSMM02]. utility [KMH02]. utilization [GS08, DMLI05]. utilizing [NYTH09, Wan09].

v [Lip00, ZZW09, GBJ03, Kri09b, PFC03, TD08]. vacancy [ZMH+09].

vacuum [BISB02]. Valence
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valinamide [HJCP01]. value [FP+06, BS+09]. values [OS06, PMPGP05]. vanadium [PV07, Tie09]. vapor [PH+08, UN+01]. variable [CSF+09, GS08, WHRG08]. variables [SR06]. variance [BLo04, LRWG03]. variate [LR06]. Variation
[AAP00, NAT07, PGG06, RAO00a, Vya01]. Variational
[MR02, AB09, Chu07, GY06, HdmS05, Hds06, HD06, RS07a, RS07b]. Variations [TG+00]. various [BL05].

v [LIP00, ZZW09, GBJ03, Kri09b, PFC03, TD08].

vacuum [BISB02]. Valence
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valinamide [HJCP01]. value [FP+06, BS+09]. values [OS06, PMPGP05]. vanadium [PV07, Tie09]. vapor [PH+08, UN+01]. variable [CSF+09, GS08, WHRG08]. variables [SR06]. variance [BLo04, LRWG03]. variate [LR06]. Variation
[AAP00, NAT07, PGG06, RAO00a, Vya01]. Variational
[MR02, AB09, Chu07, GY06, HdmS05, Hds06, HD06, RS07a, RS07b]. Variations [TG+00]. various [BL05].

v [LIP00, ZZW09, GBJ03, Kri09b, PFC03, TD08].

vacuum [BISB02]. Valence
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valinamide [HJCP01]. value [FP+06, BS+09]. values [OS06, PMPGP05]. vanadium [PV07, Tie09]. vapor [PH+08, UN+01]. variable [CSF+09, GS08, WHRG08]. variables [SR06]. variance [BLo04, LRWG03]. variate [LR06]. Variation
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[MR02, AB09, Chu07, GY06, HdmS05, Hds06, HD06, RS07a, RS07b]. Variations [TG+00]. various [BL05].
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vibrations [CPDZH08, DR09, KCL00, vE01]. vibronic [BP07, CLP+05, LC09, NRKH02, NAT07, PZWG+04, Tor02, WM04, WM01]. virtual [GFS05, KSM05, LZ05b, PRDS08, YOB+08]. virus [AJNG01, DLRZ09, KCL06]. viscosity [ZP03]. Visualization [MMP+07, RP07b, ARL01, KLY03, PGH+07]. VMD [Fraz01]. VMFCI [CCL06]. VO [PV07]. voltammetry [KJP+07]. Volume [Sta00, BVW04, LFSB03a, LFSB03b, Mue01, QNF09]. volume-preserving [QNF09]. volumes [BHH+09, Rao00b, SBLK01]. Voronoi [GHBB04, MVLG06, SBLK01]. VP1 [KCL06]. VPP700 [KSY+00]. Vpu [KF08]. vs [CXZ+09, LLKC06, MA05, SCG04, Wib04].

W [UM03, WWCC+05, MH09]. W2 [dOMSL01]. Waals [AD00, CPUGD09, GdSuM+07, Grl04, KLH+04, LS08c, VS02]. walk [CY09, CY13]. walking [BHG03]. wall [BG07]. walled [XWL+09, ZzvRSC08]. Wang [Ano06c, GHH07, JW12]. warping [JO02]. Water [LMIF06, Mor02, NK01, BLL+06, BUMCMRL00, BRLS08, BRLS12, BSH07, DLR+08, DSB+02, ES00, FG03, FKS+09, GMW08, GDV03, Go09, HM02, HRBKB03, HPL03, HFFH06, HN02, HTN03, HLMR06, ITS06, IDMC09, KFNH08, Kle02, Kla03, LPB03, MT03, MN02, MZ05, MG00, OCP02, PHJ+08, PPYS08, RR05, SO07, SSM08, SJW09, SVV+08, THHN01, UM03, VHRR07a, VHRR07b, VL00, WL09a, WD04, WDS06, KKG+05, YT03, YSJ09, Yos02, YGLvG06, ZZ04, ZCZ03, ZZ07, ZZ08, ZWP08, BA04b, WJX+08]. water-addition [RR05]. Water-assisted [BA04b, WJX+08]. water-phase [KFNH08]. WATGEN [BSH07]. Wave [BGB03, Bac04, Bac07, Bou00, GFS05, LLK06, PFB05, PSS+04, PSMB05, RLDI09, TT05, VSK+04, YH06, YLL+09]. wavefunction [IS07]. wavefunctions [BBW+08, KTM02, PJFJPRMI07]. Wavelet [CF04, ON07, QLHL09]. waves [MOP+07]. way [GZ07, HS05b, PRSMM02, VBGL+00]. weak [QTdG+08]. weakly [CPML08a, JRJ01]. web [KKG+09, GKR08, Gra07, JKI08]. Web-based [Gra07, JKI08]. web-interface [KKG+09]. WebMTA [KKG+09]. WebProp [GKR08]. Wei [Ano06c]. weight [AG00]. weighted [FS00b, HDW03]. weights [Bac04, Bac05, Bac07, Kar01]. Weinhold [GHBB04]. well [BBP09, WCK00]. well-tempered [BBP09]. where [HYA02]. which [SBH02]. Wiener [YH04]. Wiley [Bi09, Lie00, Sta00]. Wiley-VCH [Sta00]. Will [LLW+09]. Windock [HS07b]. Wind [HS07b]. Windows-based [HS07b]. wise [Nil09]. within [Der09, DFM00, GS09, KC01b, MY08b, NYTH09, NAT07, SHBD05, SPT+03]. without [AL01, Hdm05, Hs06, HD06, HZ09, Nil09, PK05, Qua07, RKA+09, TW03].
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yield [CSD05]. YL [NYK+09]. ylide [LS08b]. ylides [Mit01]. Ylidic [XDS06b]. yloxy [BE07]. Yong [Ano06c]. young [SN00, Woo01]. ytterbium [FRS05].

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 [BTP09, GPSP06, BRI+09, ESM06, FO00, PK05, ROG00, TGGP+00, TFZRG01]. Zn-biomimetic [FO08]. ZnO [HSF08]. ZnX [WWS07]. Zori [AGSFA+05]. ZPE [MGLDS00]. ZPVA [QCK01, QCK02]. zwitterionic [ROG00]. zwitterions [KL03]. zymogen [PDP02]. ZZ [CRC+08].

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