Title word cross-reference

(Φ, Ψ) [WD04]. (ϕ, ψ) [TTB01b]. −2 [ZZZ+06]. −4 [ZZZ+06]. 1 [FROD08]. 1/rp [SG01]. 12 [KGL07]. $139.00$ [Sta00]. 14 [LMGR06, ZGXX06]. 16 [HXD08]. 2 [DMC05, GdAcV+07, LW04b, LXZ06, LW06, PF06, SFC04, WDZS07, YNW05, hYDN+08, ZTS09]. 2 ≤ N ≤ 372 [Pul05]. $3 [Lip00]. 3 [BAH+02, FROD08, GDPCPU07, GdSuM+07, HP05, mJLzYL+08, KSN01, LYZ+08, MP03b, PF06, SHBD05, SFC04, TJM+03, WLL+07a, WDZS07, XLL+02, ZLY07]. 310 [JS07b]. 3d [Hol05, LD05a, Wu06, SZT08]. 4 [FHF+01, LLXS02, QB05, WDX+02]. 4, 7 [ZWS+02]. 4d [ABY+08]. 5 [ZXL+04]. 5d [HZ09]. 6 [Han01, LLXS02]. 7 [LMO09]. 8 [KS05a]. 9 [UM03]. [n] [VKP+08]. ## [BRV+07]. + [FKS+09, GLRL02, GPSP06, GWL07, HDO+02, ITS06, KT08, LMO09, Mck07b, PV07, Sha02, WWT08, ZYW+09, ZL05, dRLMS00]. +2 [PNG08]. − [Bac09, Dib05, HTN03, LYZ+08, Mas01a]. 1
[AGI+07, IS03, LDT+02a, XZ04, ZX04, ZLLS04b]. 125 [HWFN01]. 13 [FHF+01, VBS09, ZLD09]. 15 [LKA01]. 10 [FO04]. 1 Σ [BAL+01]. 1 Σ [BAL+01]. 2 [BAL+01, Gog08, PRSMM03, ZWS+02]. 2+ [AS06, BTP09, BL00, FHRR07, GSPS06, HLBO9, KRLD09, Kri08, ROGO0, TFZRG01]. 2- [IvSV06, JD09]. 2 II [Gog08]. 3 [BPC01, LDT+02b]. 3+ [BTP09, BL00, Kri09b]. 5 [VBS09, CJW+09]. • [Mui05]. ISQ [Bac09]. MTC P1 [BRDC02]. n [ZZZ+06]. p+ [GSPS06]. 0 [DLT+02]. 1 [BPC01, LDT+02, WLPF05, XWXC08, YKK09, ZZW09, XWXC08]. 103 [NSO+07]. 11 [XB08]. 12 [WZZ+09, XB08]. 141 [GYCZ04]. 18 [ZZZ+06]. 2 [Bac09, BAL+01, BL00, BBI+09, CPJ00, CCCJ09, CTFC08, DLD+02, DRAS04, DRAS05, Dib05, DMN05, Don08, FJ08, GCCVB00, GBDP05, GSPS06, HYR06, HK07, Hua09b, JPF+00, mJlZsLyL07, KZY09, KS05a, KKJH08, KBL08, KS05c, LDMR01, LC07, LWK08, LLXS02, LW04a, LZZC09, LAT05, LF02, LDT+02b, LWY+09, LMO09, MR02, Mas01a, Mas01b, MGLL03, McDO8, Mck07b, MYO8a, NA06, NYH06, NHH06, OwEO5, PGNG03, PGRRNG03, PC00, PRSMM03, PLC08, RAGLL09a, RAGLL09b, RD00, RDM+08, SLL+04a, SLL+04b, SRE08, STC+08, TJM+03, TD08, UCT+03, UTT+04, VS02, WLLS05, WDS06, WDS06, WLL07a, WDSZ07, WLL+07b, WD08, XF06, YTY07, YLW+08, YLWL09, ZY01, ZZL04, ZLLS04b, ZWL+05, ZLL06a, ZLL06b, ZKK+07, ZXY03, XZ09, dOMSL01, dRLMS01]. 20 [Ber03, CCB04, Ell07, GB02, Var09, WLPF05, WLO9b, ZZZ+06]. 2 [dOMSL01]. 2 [LMCD09]. 2+ [GHLK+02]. 2- [GYMN07]. 2 Λ [YKK09]. 3 [BPC01, CPJ00, DRAS04, DMN05, FJ08, GBDP05, GD06, HLLS05, HYA02, HD0+02, HTN03, ITS06, mJlZsLyL07, mJlZyL+08, KZY09, KT08, KJH08, KSTC01, LDMR01, LD05a, LMK01, LDC+07, LW04a, LW+06, LF02, LWY+09, MR02, Mas01a, MGLL03, Mck07b, Mui05, NA06, ON07, PGNG03, PGRRNG03, RD00, SAS05, SLL+04a, SM06, SCP08, TJM+03, TK08, TD07, UTM+02, UTT+04, VMD06, WDS06, WLL+07b, WDX+02, XS06a, XFF06, YLW+08, YLWL09, ZJM+07, ZZL04, ZLLS06a, ZZW+07, ZZL+08, ZXYF09, ZZL+09, ZKZ+07, ZWS+02, ZX08]. 3-n [mJlZyL+08, KSN01, WLO7a, WDSZ07]. 36 [CS01]. 4 [DRAS04, DMN05, IN08, IvSV06, JD09, LDMR01, LMK01, Mck07a, PHH+08, TYN05, TK08, UNM+01, UTM+02]. 4-n [FHP+01, WDX+02, XLL+02]. 5 [GD06, LYZ+08, SLL+04b, ZZL04, XWXC08]. 50 [ZZvRSC08]. 54 [GZ07]. 6 [BS01, GHLK+02, Han01, KRLD09, LDMR01, LZZC09, LAT05, LYZ+08, RPNJ07, SLL+04b, TYN05, XB08]. 6-n [Han01]. 60 [CJS+03, EI07, KJP+07, Owe05]. 62 [HK07, STC+08]. 64 [CTFC08]. 64 [CTFC08]. 64 η [HYA02, LZZC09]. 64 [GZ07, Mck07a, Mck07b, PLC08, WLL01]. 80 [KSN01]. 9 [Mck07a, Mck07b, PLC08]. 90 [NSO+07]. A [Sha02, KKS04, MK02, ZPL07]. cam [ZAT07]. carbene [HA04]. h [WLPF05]. i [OS08]. m [LYZ+08]. N [BP01, BSB05, HTN03, MG00, Owe05, RC04, YT04,

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

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

1 [AJNG01, AVS09, BPC01, BWE05, KF08, NLL+09, SPT+03, VVS07, WC09, WHF08, YT04]. 1- [CUS00]. 1-aminoo-3-propenal [FDSA00]. 1-jk [SPGS08]. 1-naphthoic [CMLS05]. 1-pK [ZCS04]. 1-X-bicyclo [BCP01]. 1.0 [AGSFA+05]. 10-endoperoxide [CG08]. 10-membered [ZW09]. 1174 [WWC+05]. 12 [HDO+02]. 12-crown-O [HDO+02]. 1291 [Ano06a]. 1328 [Ano05b]. 142 [Ano06b]. 1629 [WB04a]. 1Z [Lu09].

2 [BL08, LBG08, MM02, PFR04b, Höf05, HTN03, MG00, PO03, RC04, WC09]. 2-allyl-2 [ZGZX07]. 2-amino-2-imidazoline [XKG+05]. 2-amino-2-oxazoline [XKG+05]. 2-amino-2-thiazoline [XKG+05]. 2'-aminouracil [BL08]. 2-Aminopurine [SC01]. 2'-aminouracil [BL08]. 2'-azido-2'-deoxyribonucleoside [PFR04b]. 2-chloro-2'-deoxyguanosine [MM02]. 2'-deoxyribosel [LBG08]. 2-difluoroethane [CUS00]. 2-dihaloethanes [WFR08]. 2-dihydro-pyrimidyl [WJX+08]. 2-dimethoxethane [LCGA03]. 2-electron [ABF+03]. 2-H [LDC+07]. 2-oxazolidones [OY01]. 2-oxo-1 [WJX+08]. 2-oxoimidazoles [JKM08]. 2-phenoxycarbonylic [KKL03]. 2-substituted [OSA06, WW04]. 2-thiouacil [LMGO+09]. 2.0 [GZM09]. 21C7 [GLRL02]. 21D8 [UTH+03]. 22 [Bof01, Qua01]. 24 [Ano06b]. 25 [Kne05, WB04a, WW+05]. 26 [Ano05b]. 27
3 [AAP00, KAK+09, LEV+09, NYTH09, Rud05c]. 3-butadiene [Hir08, WR07]. 3-dihydroxy pyridine [YXZ+04]. 3-dimethyl allene [LLKC09]. 3-fluorobutanal [NSB08]. 3-hydroxy-2- mercaptopyridine [YXZ+04]. 3-trimethylsilyl-1-pyrazoline [LLKC09].

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

5 [LDY+08, PFR04b, PMM05, TAS07]. 5-di-tert-butyl-o-dimino benzosemiquinone [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].
[WD08]. **ABSINTH** [VP09]. Absolute Boundary [BWE05, ZM09, BMRF01, DHF+05]. absorption [MWL+08, MSH+06a, YXZ+04]. abstraction [AST06, CUS00, CUSS03, GAIM+01, mJZL+07, LW04a, LLL+07, TLL+07, WLL+04, XL+02]. Acceptor [GHLK+02]. accelerated [Gou07]. Accelerated Absorption [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, BMIL+04, GB04, HHS+05, LFS+07, RP07d, TSM+01, TRS+02, ZCL+09]. Accessible Surface Area [ZCL+09]. Accompanying [Ish02]. account [May07, SN06, Vya01]. Accuracy [FT+07, GG09, PSMB+05, SKK+07, UBDPJ+04, Bie+04b, FKFG+08, JS+07b, KC+01b, MKGA+06, MH+04, RK+05, SM+03, SW+06]. Accurate [ABWT+09, BDPRMAI+00, EK+06, G+09, G+04, H+06, HSM+06, Ish+04, LLZ+09, MSH+06a, Tot+04, WFHP+01, WHP+02, WHF+08, WX+09, ALKH+04, Bie+04a, BLB+09, GCBF+05, CF+06, GKK+07, H+06, J+05, J+07, J+09, KA+06, MH+04, RK+05, SM+03, SW+06]. Accurately [IGL+07, SB+08]. acetaldehyde [Lu+09, YLZ+08, Lu+09]. Acetalization [RUP+06]. acetalts [MG+06]. acetamide [CCK+01]. acetate [GWM+08, PGG+06]. acetic acid [CJK+02, CML+05, CJ+00, FM+00, HW+03, IKYM+09, KS+01a, LD+08, MB+00, MM+05, NH+05, O+08, PPYS+08, Van+02a, XKK+03, YLL+09, ZCL+09]. Acetate [GHLK+02]. acetylcholinesterase [MCK+05]. acetylcholinesterase-catalyzed [MCK+05]. acetylene [LD+02]. AcF [GHLK+02]. acid [CJ+02, CML+05, CJ+00, C+01, DP+03, DL+06, DH+07, FZ+07, HF+06, HLC+09, IT+03, IKYM+09, J+00, JKM+08, JCL+05, KLB+03, LL+07, MT+03, MML+05, MSF+08, MH+08a, Nak+07, NH+05, NLL+09, Pac+06, RR+05, RK+03, SKGS+00, SY+03, SL+04, SBO+09, SWR+06, SHK+05, UNHY+06, VM+02, XSHC+06, XLC+08, XLT+03, YT+03, YXL+09, ZZ+07, ZZZ+08, ZO+06, vDSS+04]. Acid-3 [vDSS+04]. acid-catalyzed [RR+05]. acid-nucleotide [MSF+08]. acidity [ELK+09]. acids [BE+06, CAD+03, CLA+00, FM+00, HWT+03, HP+04, IKYM+09, KSO+1a, LD+08, MB+00, MM+05, NH+05, O+08, PPYS+08, Van+02a, XKK+03, YLL+09, ZLD+09]. AcO [GHLK+02]. across [HZ+04, SSM+08, SR+06]. act [GM+01]. actinide [AB+00, GHLK+02, NSO+07, VMA+03]. Activation [EL+06, BGC+09, BLZ+05, CC+09, CF+04, KT+08, Lu+09, PV+07, RRS+06, Vya+01]. active [AG+00, BSD+04, CFR+06, CFS+09, FCP+04a, FCP+05, HBM+06, HFS+07, HYR+06, JHPRSM+05, KSK+00, KZR+03, LLL+03, MDA+08, PFM+06, RZWS+07, SS+05, SFR+07, TGD+06, XLZ+08]. active-site [SFR+07]. activities [HMM+09, MS+04, ZBW+09]. activity [AGMP+08, BOU+1, CW+02, DD+08, DA+01, DH+08, DH+09, FTL+01, GDP+08, LC+09, MRS+09, S+02, WZY+04, ZER+08]. acylation [MCK+05, MK+02]. adaptable [KF+08]. Adaptation [HLM+05]. adapted [FCP+04b, H+06, HD+06, LW+07, PTC+01]. Adapting [BB+00, HBW+01, HW+03, HLS+05, DK+01, GY+08, OM+04, RNG+03].
addition
[BLO+02, DGD+05, LL00, Mui05, RAGL+09b, RR05, WGW08, WSC09].
addition-elimination [Mui05]. additions [AVB00]. Additive
[GGK+08, CCK01, LKA01]. adenine [KKMMS04, SGO7a].
adenine-thymine [KKMMS04]. adenosine [MRS+07, YKK09]. ADF
[vTBB+01]. adiabatic [SLRC01, TVL+03]. ADMA [EM03b]. admissible
[WG02]. adrenergic [YKK09]. adsorbed [DR09, PBZ00, XPW09].
Adsorption [ATH+03, BRS00, BRS01, HSF08, ZTSP+08, NK06, SURG06,
ST04, WLX+05, ZCS04, ZSC05]. Adun [JGVF05]. advanced
[LAEL01]. advances [MMVH07]. Advancing [PP08b]. affect [AST06].
affinities [AVS09, DJ04, KS05a, KKMMS04, LXXS+02, MRS+07,
SRB06, WSM+08]. adhesion [AVS09, DJ04, KS05a, KKMMS04, LLXS02,
MRS+07, SRB06, WSM+08, ZJM+07, ZXL+04, dSGG00]. 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, SGO7a, WCS09]. against [SSS+09]. AGBNP
[GL04a]. AgBr [Sha02]. agent [LHJ+06]. agent-based [LHJ+06].
aggregate [KHF+09]. aggregates [AB08]. aggregation [IM06, OGH05].
AgN [ZG08]. agonists [GCD+08, SBG+09a]. Agreement [LS05b]. aided
[PJJ+07]. AIM [SFC04, CFS03, WW03]. AIM2000 [Ano01a, BKS02].
AIM2000-Program [BKS02]. Al
[OS08, WZZ+09, Van08, KKH08, QB05, WZZ+09]. al. [RKH03]. Ala
[PC00]. alanine
[JSR+07, ECA06, GAIMVB01, GSB09, GKT04, HHP04, HMK02, JW06,
LSW+01, MOP+07, MFR07, PFJ+03, Qua07, WD04, ZW09, ZM06].
aliphatic [RGP+07]. Alchemical [Blo04]. alcohol
[FBDG06, JHMB+09, KB02]. alcohol/water [FBDG06]. Alcohols
[ACLED03, LCGA03, LCA03]. aldehydes [LLA01d]. Alder [Hir08].
algebra [AT02]. algebraic [Tor02]. Algorithm
[GG09, GGB07, KS03, MO01, WM12, ASWG07, AM06a, AM06b,
AGSFAL05, BP02, BED02, BA08, BMT001, BSH07, BHH+09, CS02,
CLZX09, CWV+05, CF04, DDKV07, DP03, DP04, JSR+07, DBGV07,
DAK08, FKFG08, FCP+04b, GF08, GLD08, GCD04, GM04, Gou07, GKK07,
HHJ03, HH04, HM06, HLM05, Ish04, IPN06, IPN07, JCA+02, KH01, KM00,
KMA+07, KUB07, KVGH01, KH06, LJJ+07, LSJ05, LM03, LMO09, MPP03a,
MP03b, MVLG06, MM07, Nak02, OR05, PV03, Rap06, RHL09, SKSH07,
SJJ+04, SWR06, SSMW09, Ste04, SBH02, TYO+02, TGD05, VGO+07,
WRBV03, WCSS09, YK00, YGZ05, ZBS03, ZZ08, ZA07, vLBBA12].
Algorithms [LMH+09, BYQ03, BdPRMAI00, CKMC04, CSR04,
CHM+05, DB06, FSH9, FS00a, HWD03, KOFF09, OTL08, OGH05,
RLERO4a, SE08, TP01a, VW04, WK01, YL06, vLBBA12, HBW00, HBW01].
alignment [BA08, CLZX09, CLZX09, HHG+09, RI07, VGDSU08, Leh06].
alignment-free [VGDSU08]. aliphatic [MSR04, SDG01]. alkali
[JHMB+09, JHMB+11, WWT08, ZY+09]. alkalimetal [BSG07]. alkaline
[JHMB+09, JHMB+11]. alkaloid [BMRF01]. alkane [HGMB04]. alkanes
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]. AnF [Han01]. Anglada [Bof01, Qua01]. angle [CIB05, FWH+07, LI07, OFIK09, YL06]. angles [FPG+06, FKZ09, HK08c, WHRG08]. anharmonic [BP07, DB07, GBDP05, LMO09]. anilido [GTC06]. anilido-imine [GTC06]. 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]. anomic [CPJ00, CPJ01, CKF01, LCD03, 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, HMM09, KSS08, KAK+09, KBK+01, Mat03, MW09, TBSM09, TKN+08, BLN01, COS01, CSJ01, DLVW07, DV02, FOK+04, FUK+05, GLD08, GWM+00, HHHB06, JW06, JGVF05, KTM02, KOka1, LL00, LFSB03a, LFSB03b, LI07, LSHR04, LCSZ09, LXL07, LLL03, LMO09, MG00, MS04, PB04, RIO7, Rud05a, SG07b, Tot04, VM00, Wil01b, WR07, ZLY07, ZNL07, dGWH01, CMJ08, CWW+05, CMBC08, 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, ECM+03, GGB07b, HT03, RSN+02, WH03]. applied [ADM+06, BL09, BT00, BS06, DMN03, FII+07, GHLK+02, MKGA06, OM04, TLK00, YAÇ+02, ZZZ08, dVB01, BBC+05]. Applying [AGMPRG+08, Woo01, You11, GZ02]. appreciation [vRS01]. approach [AB00, AGK03, AVS09, BG03, BME05, BS03, BGJ01a, BLF02, BMTSC01, BPDC07, CCWH02, CVM02, CGBF05, CAGR08, CMBC08, CG05, EM03b, GAIMVB10, GA106, GJL+08, GRO+03, GDV03, GS02, GDPP08, GdSuM+07, GdAcV+07, GCD+08, HMM09, Hnn00, 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, VW03, Van02b, WWL+09].
XWC09, XKKL03, YS00, YK08, ZCS04, ZS04]. Approached
[LL07, XSHC06]. approaches [BP07, Con02, CSD05, COL+06, MLJ03,
PSF+08, PMM05, RL0D09, RSS09, SM08a, YCW+09]. appropriate [Bac07].
approach [Cu08, GB04, Hol05, KS02a, SZT08, SYC03]. approximated
[PSF+08]. Approximately [EA06]. approximating [MR04].
approximation [AB09, BRS00, BR01, CLP+05, CCK01, Der09, EA08,
GMA04, GWS+02, ION07, Kri09a, Lai07, LFSB03a, LFSB03b, LN01,
MTE04, Nee03, OCB02, RL07d, SHSF05, ZFL+09], approximations
[Dya02]. APS [CBC+08]. APX [ZJM+07]. aqua [RMP01]. aqua-
aque [RMP01]. aqueous [BISB02, CPJ00, CPJ01, CW02, CCK01, DA01, EK06,
FHRR07, HMWC03, HRR05, HD0+02, IV04, IvSV06, JH07b, KEH02, KPR04,
Kri09a, Kri09b, LTR+02, LR03b, Loc03, LMIF06, MM02, NL07, PK04, PHRR08,
SH09, SMK00, SBB02, VP09]. arabinonate [RGP+07].
arabinonohydroxamate [RGP+07]. arbitrary [KH06, LMV07].
architecture [TDK07]. architectures [TYY+02]. area
[GCD+08, GB04, HHS+05, Lab08, LFBSK07, RP07d, VP02, ZCL09]. areas
[BBH+09, TRS02]. arene [FKS+09, PCMG09, RRZA08]. arene-containing
[RRZA08]. arginine [CJPZ08]. arginine-bound [CJPZ08].
argon [BWW+08]. argument [Ish04]. ARIs [PS09a]. arising
[CCSJ00]. armed [KLM+09]. ArOCS [ZGXX06]. Aromatic
[CPML08b, PCO+07b, Van08, Bor03, FVBO8, HLC09, MM05, MGMM07a,
ST01, SMV+09, TDK07, VS08, WFP01, XLT07, PCO+07a].
Aromatic-Backbone [CPML08b, Van08, PCO+07b, PCO+07a].
aromatic-type [HLC09]. Aromaticity
[BPCD07, FMPS08, JHMB+09, JHMB+11, LWW+06, LTF+07, MGMM07b].
Array [FJP07]. ABF+03]. arsenic [ALC08, KS05a, ZXL+04]. ARTE
[VB07]. ARTE-QSAR [VB07]. artifacts [CCSJ00]. Artificial
[PS09a, RWBH09, dVB01, CLC03, Gol09, NINAT+07, TCSM03]. arylamide
[VIP+06]. ascorbate [HB06]. ASIC [NYTH09]. aspartic [ZZY08].
Aspects [HBBH00, MO01, BMRRB01, BR07, Sie01, TT02]. assemblies
[DFG09b]. assembly [DPP05]. Assessing [IB04, FG07]. Assessment
[BP03, CCW02, DGI+08, KS08, LW06, SS+09, WSM+08, CKMC04,
FMPS08, GTO3, LLS03, SP05, GGT08, GBB04, TFZRG01]. assignment
[BB05, BMRF01, PRJ02]. assignments [PS06]. assisted
[BA04b, KT08, WJX+08]. assists [BM07]. associated [SWR06, TT08].
Associated [ABYMO8, NL08]. asymmetric [WR07, WFR08].
Asynchronous [GLP08]. atmospheric [GCCVB00, PGN03]. Atom
[RP07a, RM00, BPC01, BR04, BWW+08, CCK01, FM00, GW+02, GB04,
HLS05, IT03, JS07a, mLZL+08, LMK01, MT03, MB00, PHH+08, RG08,
RS08, SBB+03, SBLK01, SLL+04a, TG07, V0K6, VGO+07, WLL07a,
WBSR03, WS07, WLL+03, YLWL09]. atom-bond [VK06]. atom-centered
[SBB+03]. Atomic [DVP+02, FDM00, AS00, BAC07, BSC+01, BCNS07,
BSP06b, BK00, BLT03, BAA07, CN03, FS04, GC02, Ish03, JBB00, JBB02,
KRM+02, Kau07, KS01a, KCO1b, Lab08, LM07, LST08, LTVO8, NIO09,
atomic-centered [TBSM09]. atomistic [CA04, IDMC09, KK01b, 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, Wil01b, WDX+02, XLT07, YOB+08, dSGCG00, DVRP+03].

atomic [TBSM09]. atomistic [CA04, IDMC09, KK01b, 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, Wil01b, WDX+02, XLT07, YOB+08, dSGCG00, DVRP+03].

atomic-centered [TBSM09]. atomistic [CA04, IDMC09, KK01b, 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, Wil01b, WDX+02, XLT07, YOB+08, dSGCG00, DVRP+03].
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, IKK09, IR03, JD09, JKI08, JGF05, KLS02, KBA+04, KK08c, KBB+01, Kob03, KIM+09, KZW+09, KVS+06, LFKL00, LHJ+06, Leh06, LXZ06, LJZ+07, LH05, LM09, ML06, MSF+08, MUR+06, MBH02, NLL+09, NMAT01, OVMV04, PS09a, PFR04b, PA05, PA07, PR02, PF06, PRDS08, Pul05, QHL09, Ra00b, RX07, RSER09, RH09, RSS09, Ru07, SAM06, SKSH07, SG0809, SPM+02, SB02, SE08]. based [SZW+05, TTM09, Tot04, VSK+04, VB09, VGSU08, WL09a, WL00, WS07, WRBV03, XY+06, XL02, YWH05, hYM+08, YJF06, YXL+09, YKK09, ZCL09, ZLY07, ZLD09, ZWB09, dSR08].

basic [BCP03].

basicity [EK06, Lee09]. bases [CCK01, Nak07, RTG00, RKH03, SL04, WRP06]. basic [Rud05a]. basicity [EK06, Lee09]. Basis [AHK02, MV06, Pen06, VKCK09]. Benchmarking [Hol05, SZT08, WS07]. Bennett [KBB09]. Benzdiynes [ASY01]. benzene [BE09, BRLS08, BRLS12, HT05, HRG07, IINK09, LWX07, Sch00, SG07b, ZTP+08]. benzene [PB05, WRP+06]. benzo [GLRL02]. benzylic [BWR00]. Benzylpenicillin [DSS03]. Beowulf [BMRDB01]. Bergman [PWFS01]. Besalú [Bo01, Qua01]. Bessel [DBS08]. Betaine [LI09, BTP09]. Betaine [LI09]. between [AD00, AZM03, BPS03, CFR06, DRAS05, EQFD09, FG03, FL07, FO08, FKM+06, FKM+07, GWM08, HPP00, HRB03, HFHL06, HN02, Hir08, IINK09, JPC08, KWK+01, KWK+02, LDC+07, L01, L01, LFZ04, L0L03, LS05b, MST+08, MBH+02, OY01, PSF+08, PMPGP05, PS03, RLR01, SM08a, SBKL01, Sim07, SWM04, SKK+07, SP05, TYN05, TK08, TDH06, UTM+02, UTU+04, WLX+05, YT03, YQQH09, Yos02, ZZTS09]. beyond [CLP+05, CCK01, Haf08, PP08b]. BH [QZL+04, SAS05]. Bi [LS08a, WL09b, HZ09]. bi-transition [WL09b]. bias [OM04, SY09]. Biased [MLG04, KV00]. bicyclic [EBDP00]. bicyclic [BE07, BPC01]. 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, BSP06b, DLRZ09, Dra00, ECM+03, FKV+05, GCD+08, GS04, HT05, HNW07, HNW12, IO08, JMD+02, JZD+09, KFB05, KS08, LXW+09, MK02, MIJS06, MLL+08b, MRS+07, NyHN06, NIH06, OYH09, OFIK09, PMGL03, RSP03, RG08, RK05, Ru07, SOOF05, STSF02, SWV+05, TGGP+00, VGGMM05, WM04, WHF08, Wou00, 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, WB04b, 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]. bishomoaromaticity [HWGB01]. bisphosphatase [MRS+07]. bispidine [ACM+06]. bits [PM02]. black [MBP09]. Blind [GZM09]. block [ATM+07, ASS+02]. blocked [RRS09]. blockers [HSMT04]. blocks [SB+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, Lo03, SM03, TKH07, LR03b]. Bofill [Qua01]. Boltzmann [WB04a, WB05, ABWT09, BW00, BBP09, BH03, BF04, BF07, GP01, GCD+08, GGT08, HRS+05, HBW00, HWW01, KWWH07, LDG02, NYTH09, PZ04, SAT004, SZM+08, WB04b]. Bond

[CGMPT+08, CRC+08, JG03, MGCA07, May07, SH08, WM12, Bic09, BL06, CMLS05, CPFL02, CPDZH08, CJW+09, Cul08, DR09, DGD+05, DMZT08, FH01, FO08, GYMN07, GR07, GS07, HRG07, HS07a, Hir08, JPCA08, JP09, Kle03, KBLP09, LC07, LZC09, LSO8c, LS05b, MG00, OO04, Pao06, PSC+01, PAS07, PYS05, PV07, Rao00a, RM07, RCJ02a, RD00, SEKS09, Sha07, Sim07, SPT+03, SWZ04, SMZ05, SMW09, ST01, SSW+07, Tjm+03, Tru07, VK06, VBGL+00, WHRG08, WJ00, XWXC08, vLBBR12].

Bond-based [CGMPT+08]. bond-order [LS08c]. bonded

[CPDZH08, Gon07, HT03, IO08, LB05, LD+09, LZF+09, McD08, MH08a, NBTN04a, NBTN04b, NL08, PHFC04, ZH08, vEMK01, vE01]. bonding [AM07, AG00, Bac04, Bac05, Bac07, BHTCG07, BM07, BSG07, CWWS07,
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, XK08, Yos02, ZX04, ZW09, ZB07]. bonds
[Bac05, BUMCMRL00, BRS07, CRC+08, DR07, HA04, Mit01, NHH05, OO08, PG06, PC05, PC07, SO09, SGD06, SJW09, YT04].

Book
[Bic09, Lip00, Sta00, Woo01].

borane
[ZZZ+06].

borate
[HT05].

Born
[LFSB03a, BC06, CF06, DLG00, FOL+04, FC06, GZL02, ILB03, Lab08, LFSB03b, MTE04, MCM04, OCB02, Tot04, XL02, YJF06, ZGFL01, ZWZ09].

Born/volume
[Lab08].

borohydride
[QZL+04].

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

Boron-doped
[JBGK08, LWLS07].

boronyls
[LMGR05].

BOSS
[JTR05].

both
[HdMdS05, HdS06, HD06].

bound
ˇCJPZS08, WC09].

Boundary
[BH03, ABWT09, Ara04, BVW04, BF04, BF07, HH04, KWHH07, QSS01, TK08, WM06].

bovine
[MBC08].

bowls
[LMGR06].

box
[LM03, WM06].

box-counting-based
[LM03].

boxes
[MBP09].

Boyd
[Sta00].

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

brain
[CRGN07, HMSM06].

BrCl
[WLLS05].

breakage
[SWR06].

breakage/closure
[SWR06].

breaking
[HRR05, Pac06, VHRR07b].

breast
[VGDSU08].

Breit
[Ish03].

bridge
[CFC+08, PAS07].

bridged
[LHP01, SMM+08].

bridges
[KF03].

built
[GFS05].

bulk
[BACJCT01, BGC+09, EBL+08, JBGK08, LZZC09, LLL03, PB04].

bulk-doping
[JBGK08].

butadiene
[GRO+03, Hr08, WR07].

butanal
[NSB08].

butanes
[WW04].

butyl
[Bac09].

C
[Ano00, BAL+01, BPC01, BSB05, Bac09, CTFC08, HK07, mJlZyL+08, KF07, KJP+07, KSN01, LYZ+08, Mck07a, Mck07b, Owe05, SLL+04b, VBS09, WLL01, WDXS06, WZZ+09, XFF06, YHD+06, ATBLS04, Ber03, CPDZH08, CCB04, CS01, CRSB03, CTFC08, DGD+05, DRAS04, EL07, FHF+01, GYCY04, GZ07, GB02, HBM06, HYA02, HK07, HA04, IN08, LDMR01, LMK01, Mit01, O004, PRSM03, PV07, RD00, RFSS06, SLL+04b, STC+08, TYN05, WLPF05, WDXS06, Wil01b, XDS06a, WXWC08, ZZZC09, ZL09b, ZZvRSC08, dRLMS00].

C-PCM
[CRSB03].

C12A
[BRDC02].

C12A-p8
[BRDC02].

C96
[ONHN00].

Ca
[WZ+09, WD08, XWC09, Hlb09, PNG08].

cabonyl
[RUPH06].

CaCO
[SCP08].

cage
[CS01, KFD06, WLPF05, WLO9b].

cages
[CJS+03, Wan09].

calcium
[HSMI04, HLB09, LGB+09, MHJS06].

calcium-induced
calculate [BACJCT01, CSD04, IS07, Kar01, Kne05, KBLP09, OV03, RSNN02, SFRS01, WW03, YS00]. calculated [BE06, BE07, GG09, Gra07, LMV07, RSKK03, RM00, Wib04, WM04, ZXY08, Klee03]. calculates [ATMK03]. Calculating [Chal07, CG05, DRMD03, DF04, LN01, MC06, PDC+08, PMM05, RSE07, SYC03, WCK00]. Calculation [BK00, CPML08a, DJ04, KKY01, KRM+02, LSW+01, MT03, MO01, MRS+07, TS05, VM02, VC04, WKYY01, ZWPR+04, BP02, BSBC+01, BH03, ECA06, FOL+04, FR0D08, GKR0G08, GLMV09, GAdGM08, GGT08, HTKG08, II02, ITN+05, JJK+00, KFNN08, LFK05, Li01, LLZL09, MGLO03, NRK0H2, Nil09, OCP04, PZWG+04, PR SVM08, RNG03, Rap06, RLER04a, RKA+09, RRFC+03, SOOF05, STSF02, SSM08, SHH07, TZX01b, TZX01a, TLOG00, TPR01b, TRS02, TKN+08, UKN04, UHH09, WLLS05, WLL+07b, WSM+08, WM01, XOW+00, ZWB09, ZL09b]. Calculations [YH07, An01b, ALKH04, Bac09, BP07, BSBF05, BMRDB01, Bl004, BMM07, BMRF01, BIV+02, CLP09, CMJ08, CN03, CRS05, Chi01, CS03, CMA+08, DB07, DPDG05, DSS03, DMV05, DPC+08, EBL+08, EL09, FKFG08, FL08, FMSA06, FR06, FO04, GJL+08, GBDP05, GM04, GWM+00, GGB07, GPSP06, HHBB00, HLLN06, HAY02, HMSM06, HFHL06, HKHN08, HT03, HWGB01, HZ09, Hua09a, Hua09b, ILKR09, IPN07, IPN07, JCA+02, JBGK08, JCHS07, KGL07, KWHH07, KRLD09, KTM02, Kob03, KBLP09, KS02b, KKS04, LLA01a, LLA01b, LLA01c, LLA01d, LLQA03, LSFB03b, LDC+07, LH09, LW060, LC06, LK0W04, LZF+09, LS05b, LD0G02, LMO09, MMLC05, Maa08, MBC+00, MA05, MLCD01, MLJ03, MS01, Mui05, NYK+09, NTH09, NSU+02, OBB05, OYH05, OS06, OKH+02, Oos09, OKE+02, PB06, PMLG03, PVdJJ00, PV03]. calculations [PBZ00, PRSM02, PSS+04, PSMB05, RSP03, RPM01, RP02, RRCA08, ROC00, RWBB09, RS05, RRS07, RJLR06, SB08, SSB+03, SCS07, SGB+09a, SHM04, Sha02, SSL02, SNS06, SFRS01, SMG09, SG01, TK08, TY03, UKNS01, UTM+02, VKP+08, VZVG06, Van02b, Ve09, VIP+06, WL02, WTKM06, W08, WC04, WHF08, WR07, WFR08, WHG+07, WJ00, XLZ08, YTH01, Y08, YSA+03, ZSE08, ZXY09, ZM03, vGBB00, vdVGDJ00, LSFB03a]. Calibration [OKH+02, LLZL09]. calix [RRZA08]. camphor [AST06]. Car [DSB+02, DDBP09, LC07, MSH+06b, PB06, SBI08, STSF02, WS07, IGL07, Mck07a, WCF04]. cancer [VGSU08]. Candida [RGPP+07]. candidate [SF07]. canonical [BP02, EMP07, ITN+05, IS07, KM00, KN01]. CAOs [PS03]. capabilities [GCCD04]. capped [ZC03]. capsid [KCL06]. captopril [AG0+02, APG05]. capture [YXC+07]. Car [JP09, Sch04]. carbapenem [BBSS06]. carbenes [HA04]. Carbohydrate [KBN02]. carbohydrates [ACLD03, HR08, KDSV02, LR03a, LCDA03, LCAG03, LCA03, LH05, MW00, Sto05, KYT+08]. Carbon [KK08c, LMGR05, BS05, BG07, CZ05, CDPL09, DWS+09, GKK07, HT05, KT08, KLS02, KKO1b, LMK01, MMRVH07, PAS07, wQZSLyZ02, SRS07, Wan09, WSC09, XWL+09, ZKZ+07, ZYW+09, ZZvRSC08]. carbon- [ZYW+09]. carbon-centered [WSC09]. carbon-rich [CZ05]. carbonate
[vDSSvA04]. Carbonyl
[RD00, DLR+08, LL00, LL01a, LL01b, LL01c, LL01d, LL03].
carboxyls [BRV+07, LMGR+05, PLC08]. carboplatin [WM01].
carboranes [JR01, OSA06]. carboxybenzisoxazole [UTH+03].
carboxylates [ČJPZS08]. CarC [BBS06]. carcinogenic [EL06].
carcinogenicity [VS08]. Carlo [AGSFAL05, AGSFA+05, BR03, BHG03, Der00, FCK+08, FKFG08, 
GH07, HMD06, IN06, IKYM09, KLS02, KM07, KKC05, LML+00, LZA02, 
LWG03, MH09, Nak02, NA06, NCO+05, OM04, SKGS00, SCS07, SBJ08, 
SM08, SWR06, TS05, XKG+05, ZCS04]. Carlo-with-Minimization
[NCO+05]. carma [Gly06]. carrying [Tor02]. Cartesian [LPK07, PHR+05].
CAS [PRSMM03, BMB07, JHPRSM+05, PRSMM02]. CAS-SCF
[JHPRSM+05]. CAS-SDCI [BMB07, PRSMM02]. case [AB00, AS00, 
BUMCMRL00, BWW+08, BS06, CFSS+08, ČJPZS08, MV06, MID04, Pac06, 
PBG06, PC00, Pog03, RUPH06, SBI08, SN06, Van02a, WRGB03]. cases
[BCF+09]. CASPT [PO03]. CASPT2 [KRLD09]. CASCCF
[Bac04, Bac07, DOSG06, WLZ+07, dSVA+09]. CASCCF/CASPT2
[WLZ+07]. Catalysis
[UTH+03, DWS+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, GVTG03, GLH+08, HSWW00, MCK05, OY01, 
PHG07, RR05, Sie01, TH02, TGLL07, WCW08, WCHW09, ZWS+09].
catastrophe [PA05]. cathepsin [ZWB09]. cation
[DSB+02, Don08, LB08, OO04, PV07, QZL+04, SLRC01, VL00, WLZ+07, WSM+08, Wou00, ZL05].
cation-water [DSB+02]. Cationic [JRJ01, TBG00]. cations
[ALC08, GS09, GS04, GWL07, HIA03, Ho05, NS08, RRS06, SZT08, 
WWT08, ZYW+09]. caused [LPK07, TT08]. cavities
[BCIB05, BHH+09, IME02]. cavity [RRZA08, ZFL+05]. C — [CWJ+09].
CBr [FHF+01], cc [Wib04, GYM07]. CCH [ZKZ+07]. CCl
[FHF+01, WDSZ07]. cclib [OTL08]. CCN [JDWS06]. CCSD
[BBI+09, Lu09, POF+03, PV03]. Cd [GPS06, XB08, BMRF01, BBI+09].
CD38 [UNHYT06]. CDOCKER [WRBV03]. Ce [SNM+06]. Ceccarelli
[Ano06b]. cell [Gon07, KVS+06, KS05c, LEV+09]. cell-based [Gon07]. cells
[CJ09]. cellular [XWC09]. CeN [VP08]. centauric [PA05]. center
[BR507, GA00, IN01, LA07, GM07a, GM07b, NR04, ON01, 
SPS09, TBG00]. centered [CC01, SS03, TBMS09, WSC09]. centers
[GY07, JKL08]. central [CGMP+08, CM09]. CeO [CCJ09]. ceramic
[HZX04]. cesium [HD06]. CF [mJZsLy07, LDC+07, gTHJ+01, UTM+02, 
UTT+04, WLL+07b, YLW+08, YLWL09]. CFCI [mJZsLy07]. CFF91
[TTB01a]. CFMC [NCO+05]. CH
[CPJ00, GBDP05, HTN03, IN08, mJZsLy+08, LW04a, LDT+02b, MG03, 
Mu05, RD00, SSL+04a, TJM+03, WLT+06, WLL+07b, WDX+02, YLW+08, 
ZZL04, ZZW+07, ZZL+08, ZZL+09, HKHN08, FHF+01, GD06, HLL05, 
mJZsLy07, mJZsLy+08, KZY09, KJKH08, LW04a, LWY+09, MM05, Mas01b,
chain [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chairs [Cri04, CA07b, DLHC06, MMLC05, MSR04, VM02, XLT07, ZM06]. chairs [RP09]. challenge [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. challenges [Cri04, CA07b, DLHC06, MMLC05, MSR04, VM02, XLT07, ZM06]. challenges [RP09]. character [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. characteristics [Cri04, CA07b, DLHC06, MMLC05, MSR04, VM02, XLT07, ZM06]. characteristics [RP09]. characterize [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. charge-based [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. charge-density [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. charge-scaling [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chaotropic [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chaotropic [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chemically [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chemically [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chemically [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chemically [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chemically [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chemically [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chemically [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chemically [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06]. chemically [BHG03, DLW06, Der09, Din00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kró03, LL01a, LL01, MT03, PFC03, SMG09, TGB00, SWR06].
chemicals [CMGDAC+07]. chemisorption [KKJH08]. Chemist [SH08, Bic09, Gan09]. Chemistry [Duk01, EA08]. Chemistry [Ano05b, Ano06a, Ano06c, GBL+05, vRS98, WB04a, WWC+05, Woo01, You11, tVBB+01, APG05, BWM+09, BT00, BMRDB01, BS06, BSJ01, CMAGL+04, CFS+08, CPUGD09, CMGDAC+07, CMCB08, CMA+08, DBM03, FJP07, FKRE08, GDPCPU07, GDPP08, GdSuM+07, GdAcV+07, KSB+02, KBA+04, KJVW08, KLY03, KC01a, LX07, MGCA07, MR09, MBF09, MMRVH07, MPF00, Nye07, OTL08, SH07, Sha07, SBB02, SGD06, TKB07, Vis02, Ano01c, Ano04b, LB99, Lip00, Sta00]. chemistry-based [SBB02]. chemists [Pra01]. Chemometric [HPL03, MRS09]. chemometrics [BLF02]. chemotaxis [FC06]. CheY [CMGDAC+07]. CHF [UTT+04]. CHFOCHF [YLWL09]. Chichester [Lip00]. chief [Lip00]. CHIMERA [NSU+02, PGH+04]. chip [Höf05]. Chiral [ZPL07, CGMPT+08, Sza08, ZOJ+06]. chirality [CGMPT+08, PDC+08]. chiraly [ST04]. chlorinated [DA01, WDZS07]. chlorine [mJlZsLyL07, mJlZyL+08, WLL07a, XLL+02]. chloro [JKM08]. chloroform [CCK01]. chloroform/water [CCK01]. chromium [RRS06]. chlorophylls [LKT04]. Choice [Duk01]. Cholesky [SKDO08]. chorismate [HHBH00]. chromophore [DHM+03, HFS+07, KHF+09, XZ05]. Chun [Ano06c]. CI [Ano01b, DHM+05, 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, hYDN+08, Car02, PCS04]. classes [CLF+09, HK06, QHL09, XSHC06, XLC08, XWC09]. Classic [SRE08]. Classical [ATBS04, COL+06, DK01, LLM09, MA05, Nil09, RP07a, STH02, 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 [AHKG09, Cri04, BR04, BPG01a, BWI+02, IN08, JB08, KKJH08, KSTC01, LM02, LWX07, LYS08, Mck07a, MS01, Mor02, NK06, PSF+08, SSB07, VDM06, WKY01, Whe08, WJ+08]. cluster-continuum [WJ+08]. cluster/adsorbate [BWI+02]. clustered [FPN+05]. clustering [CCWH02, FKZ09, LZ05a, LOL+08, RLA01, ZS04]. clusters [BP00, BACJCT01, CCG06, CAG07, DSB+02, GBBH09, HXD08, HYR06, JHMB+09, JHMB+11, JG03, KGL07, KDG+09, KZW+05, LML+00, LWL07, LJS05, Mck07a, Mck07b, NJ04, OS03, OS08, PBZ00, Pulk05, QB05, SCC04, SYC08, SW06, WLL01, WZZ+09, WSC09, XZ04, YCS07, ZLJS03, ZXL+04, ZWC+09, ZXY03, ZGXX06, ZX09, ZB07, Est07]. CM1
Coarse-graining [UDPJO4]. Coarse [CA07a, EBAN07, VTT+08, CP09, DR07, DJB02, HXLS09, MBC08, PSHP08, SB08, WWL+09]. Coarse-grained [VTT+08, CP09, DJB02, HXLS09, MBC08, SB08, WWL+09].

Coarse-graining [CA07a, EBAN07]. coastline [UTH+03]. cobalamin [KPZK06]. cobalt [LMIF06]. cocaine [ZDS+05]. cocrystals [CWV+05]. code [BDW00, FROD08, GBL+05, GY08, PZWG+04]. codification [CGMPT+08]. coding [LCSZ09]. coefficient [CSB+03, YSJ09]. coefficients [CCK01, DA01, GS09, Gol09, LZZC09, Whe08]. coenzyme [WC08]. cofactor [Mck07a, Mck07b]. cofactors [Ano06b, CPM03].

Cohesive [VP08]. coil [OCP02]. coiled [OCP02]. coiled-coil [OCP02]. collagen [PP08a, PRKP05]. collagen-like [PRKP05]. collapse [Mei02].

Colle [IKN08]. collections [CDD+02]. Collective [CCSJO0, HSWN01, LV08, SWR06]. collide [CKF01]. collinear [Van02b]. collision [VW00, VW04, TYN05]. Collisions [Pan07]. collocated [CJD09]. collocation [CR08]. collocation-based [CR08]. colony [CLZ+09, CLX09]. comb [LAEL01]. comb-like [LAEL01]. Combination [MI08b, DLD+02, HGH07, HSWN01, KKS04, SRO8]. combinations [ZOJ+06]. combinatorial [AL01, GD09]. Combined [CYM02, GWM08, KBLP09, RG02, ZKZ+07, BNE07, BME05, COS01, DPT03, Der09, FSFK05, KH01, KM00, LMCD09, MC06, Oos09, TCR+02, VMF+03, WX09, XLZ08]. Combining [MB08, SS00, HTK08, KN04, LLZ09, ZM09, KKK08b, LEK07].

comblike [LZA02, ZALMG03]. CoMFA [JFG04]. Comment [CPM08b, JW12, Kne05, Qua01, Van08, Bof01, CSD05, WM12, vLBMR12]. Comments [MBP09]. Common [ZAT07]. commonly [ESP04, SCF+09].

Comp [HNF012, Kne05]. compact [Kri09a]. comparably [PB02]. Comparative [CCP04, GHL+02, LS02, SB08, SCF+09, Sto05, VMA03, CMD+04, FC06, FO08, GM01, HLMR06, JFG04, KS01b, LPK07, Mc08, PKG07, PPM05, TBG00, WC09, EBL+08, JHZ09]. compared [IO08, JCHS07]. Comparing [JCL05]. Comparison [AEE+03, Bou00, CV09, DB07, DLG00, GGLR00, Kr03, SL06, SDL07, TCR+02, WMGK07, WMM03, YLL+09, ZCL09, AE06, BL05, FOL+04, FDS00, GDPCPU07, Gra07, HRRKB03, JARM02, LC07, LOL+08, LZF+09, MZ05, MS00, MTS+08, MC06, PK04, PS03, RDM+08, SBLK01, SBL05, SBB07, WB04a, WB04b, WB05, BRDC02, CTT+03, COL+06, LT04, NCO+05, ONN00, PSF+08, SPD01, SL04, SKK+07, WMW04, YKK09, ZGFL01, ZOJ+06]. Comparisons [GPK05]. COMPASS [MSR04]. compatible [BSDM04, KH06]. competing [HA04]. competitive [FG03]. complementarity [EKB02b]. Complete [BT00, MLL+08b, Pog03, PRT+07, PRT+08, MC06, Var09, WMRW+01].

completeness [AHK02, MV06]. completeness-optimized [MV06].
Complex [DFGB09, AS06, Bac09, BRS00, BRS01, GC04, HDF+07, HDF08, HMK20, IV04, IvSV06, Ish04, JLFH03, Kle02, KVS06, LB05, LDL+09, MM03, MCF05, MY08b, MY08a, NHN06, Pac06, ZWB09].

complexation [AGI07, 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, FR05, FO08, FRLN09, FKŠ+09, GTC06, GL04b, GM01, GPSP06, GPK05, Gri04, GZM09, GWL07, HLLN06, HRG07, IN08, IO08, IGL07, JMD+02, JD09, JC07, KRM+02, KJP07, LL00, LJH+06, LPP06, LH02, LMGR06, LLS03, LMMW04, LWZ09, LZF+09, LS05b, Mas04, McD08, MHOJ06, MSBS01, MLL08b, NYHN06, NR04, NMAT01, PGG06, QTdG+08, RPN07, RMP01, RRFC+03, SG07a, SCF09, SBH02, ST06, SYY+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, ZX05].

compounds [ACLD03, BB08, BLO+02, CYM02, DA01, EDAJ04, EBD+01, FJ08, FROD08, FO04, G09, Gor01, JLFH03, KFD06, LLA01a, LLA01b, LLA01c, LLA03, LD05a, LWK08, LTF+07, LW06, LCA03, LCGA03, LCA03, LJZ+07, LL09, MD04, NBNT04a, NBNT04b, PZWG+04, PYCD03, POJ01, RUPH06, SJJ+04, ST01, TTB09, YCW+09, YSA+03].

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

compression [BG07, MBWP03].

comprising [Rud05b, Rud05c].

Comput [Bof01, Qua01, Van08].

Computation [BLL+06, Car02, CD+02, FZL07, GS09, LFEdL06, TNS00, ATM03, G07, NKS02, PAS08, RK05, WZXY07, ZCZ03, vW06].

Computational [Ano01c, Ano04b, Ano05b, Ano06a, Ano06b, Ano06c, BLMS08, CZ05, CPUGD09, CMGDAC+07, CMCB08, CG05, CA07b, GBL+05, GDPCPU07, GdSuM+07, HMK20, KJK+04, LB09, Lip00, MW00, MFR07, OY03, Pac06, SPG08, vRS98, Sta00, TMBM02, WB04a, WWC+05, WWK08, Y011, Z0J+06, ZWB09, Bac04, BG00, BAL+01, BTP09, BMR01, BZL05, CML05, CFS+08, CBC+08, CJS+03, CRH+07, FG03, FJP07, FD03, FKRE08, G09, GD09, GDP08, GdAcV+07, GGB07a, KLY03, MCF07, MC03, MO8a, OTL08, OY01, OSA06, Pan07, PPM05, PWFS01, PR04, RGG08, SF07, SM03, STC08, TD08, Vis02, VZM+08, WSM+09, WOC+03, YT03, YT04, YDNS06, ZZ08, ZGZ07, ZTP+08, ZM06, Woo01].

Computationally [KM00, KFZ03].

Computations [Bou01, Dib05, CLP+05, GPK05, Lu09, ME06, Pog06, SMZ05, TT08].

compute [BDW00, RKA+09].

computed [PFJ+03, PK05, TD06].

computer [HFSD03, H505, NK01, PPXP01, PHJ+08, TRS02, UIHN09].
VB07, VKCK09, YNZ+08, Zer08]. Computing [HHW+03, WL00, BHH+09, DGRH02, DP04, DK01, GLD08, HHS+05, KFB05, LM03, MA09, ZP03].

CONAN [SSHT03]. concave [Won09]. concentration [GGT08]. concept [LSY02, Rao00b, Rud05a]. Conceptual [VB09]. Concerning [FG03, Bor03].

collected [LFS+07, Mck07b, NSB08, LLKC06]. condensed [CLP09, DGI+08, DMC+03, FM00, GLMV09, Mor02, SDvG01, ZSK07].

condensed-phase [DWC+03]. condition [SK08]. conditions [BVW04, CEP07, HH04, WM06]. Condon [Ama02a, LMCD09, TP01b].

conductor [DHW+00, FZL+06]. conductor-like [DHW+00, FZL+06]. Configuration [SLRC01, ASS+02, BMRF01, DLD+02, KBT03, LWX07, MLL06, PRSM02, PRSMV08, SSL02, SWZS04, LSAS01].

configuration [HDF+07, HTKG08]. configurations [MM03, MABM09].

Conformation [GS04, BY06, BR03, BLB09, DPM09, LXL07, PFJ+03, YL06, YZ06].

Conformation-dependent [GS04]. Conformational [AJNG01, AZS+04, BLF02, DSS03, HW09, KO09, LRI+02, LGB+09, OYK+09, OM04, PSDM00, SH09, SMGE08, SSHT03, SR09, TTBO1a, TTBO1b, WHRG08, WW04, BISB02, BMTSC01, BAH+02, CN03, CSJ01, CvG08, CS01, CCP04, CSROt04, CKT+08, DDKV07, JER+07, ECA06, FGR07, FC06, FZL+06, GMR+03, GT03, GS09, HYA02, IB04, IZA06, JW06, JO02, KB02, KK08a, KH01, Kle02, KK01a, KF08, LFKL00, LKJ+04, LCL05, LJKL08, MFB04, Mak08, MH08b, MA05, MGJAARC00, NKIS02, OML+00, OGH05, PRT+07, PRT+08, SPL+02, SWB08, SHBD05, SD09, SSBE06, WCK00, YXL+09, ZAO7, CG03, HJCP01, JPF+00]. Conformations [NHH05, CLWL09, CI05, yCkHmY08, DBM03, ENM+04, FWH+07, GBB07, GB04, HDO+02, HP05, LKZT04, MW00, OFB08, OKH+02, PC00, PFC03, Rao00b, RP09, TLK070].

conformers [HS00, HHP04, KAS+07, PG01, RSSK03, TT02, WD04, YXL+09]. Congo [SRK+00]. conical [IK00]. conjecture [Pog03]. conjugated [BG00, CZ05, DDBP09, LYS08, LC09, LFR07, WJ00]. connectivity [EDAJ04, Pog06]. conquer [AKN07, MLJ03, vdVGDJ00]. consensus [GP06, JMD+02, LLL+08, RHL09]. Consequences [RSS09].

considerations [GRCD01, PB05]. Consistent [RP02, BWT+02, ECM+03, KK08a, KB02, NUH02, SMD02, VTT+08, WM04, XL02]. Constant [MCM04, DRMD03, Sch00, VAS02, WLLS05, WLL+07b].

constants [Chu07, FCW06, GGB07a, GGB07b, HWFN01, JHZ09, Kle03, MMLC05, MGLL03, MDI04, PJPDPRM07, RRFC+03, SLL+04b, SFRS01, TLOG00, WDX+02, WZXY07, XZ08]. constrained [COS01, C06, LFKL00, MM00]. Constraining [AM09, HSWW00].

constraint [BL09, FS98, FS00a, KVGH01, YXC+07]. constraints [BVW04, Bu07, BRS00, BRS01, ECA06, Pen06, PJB+07, VMF+03]. constructed [Gri06, YCS07]. Constructing [ZBS03]. construction [HH04, RSN+02, TYO+02, UIHN09]. contact [ENM+04]. contained [LH02, SH07]. containing
counting [HYT05, LM03]. Coupled
[BSP06b, MO01, CXZ+09, DOSG06, IN08, KSTC01, LMJ02, LYS08, PSF+08, SSB07, WKYU01, Whe08, XWC09, SMAvV00]. coupled-cluster
[IN08, KSTC01, Whe08].
couplings [BPC01, NR04, TP01b].

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, BAA07, CRC+08, CKMC04, FMPS08, LFR+04, MP03b].
cross [Gal09, MY08b, MY08a]. crosscorrelation [HWDB03]. crossed [BAL+01].
crossing [LI07]. crossings [LSG06]. crossover [KRLD09]. crown
[GLRL02, HDO+02, LWW+06, ZWY+09]. crown-shaped [LWW+06].
cryogenic [HN02]. cryptand [WWT08].
Crystalline [AS00, CADW03, JB04, PZWG+04, Wil01a, ZLD09].
crystallographic [RON02]. crystals [BCF+09, CC07, F ´A01a, GAdGM08, GBJ03, PMC+08, WMS06, Wil01b].
Cs [GWL07]. CSA [NCO+05]. CSOV
[GPS06, PMPGP05]. Cu
[BTP09, GPS06, Sha02, HSF08, NK06, TDK07, WCS09, ZTP+08]. CuN
[ZX08]. cuprates [MD04]. Current [NYTH09, CDPL09, Vis02]. curvature
[TRS02]. curved [ABW09]. 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 [WCW08]. cyanomethyldyne
[WDS06]. cycle [ZAT07]. Cyclic [KJP+07, BGJ01a, CLA+00, KFM+06, FKM+07, JBGK08, LXL07, OYK+09, VVS07, WOC+03].
cyclo-AMP [FKM+06, FKM+07]. cyclization [PWFS01]. cyclizations [SGS03].
cyclo [TDK07]. cyclo-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, MH08, MH08a, SBI08, SG07a, SC01].
cytosine- [MH05]. cytosine-5-acetic [MH08a]. CZ [CRC+08].

D [IS03, PF06, SHBD05, AGO+02, BAH+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, MMP+07, PFJ+03, PF06, RLA01, RRS07, RRS09, RON02, SY09, SFC04, WG02]. database [DPM09, LFKL00]. databases [BR07, PPXP01]. dative [FH01]. David [Woo01, Ano05b]. day [GR07]. DD [ZLY07]. DD-curves [ZLY07]. Dead [YFS07, 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 [RPN07]. decomposable [VZM+08]. decomposition [BM07, CBH+03, FKP07a, FPG+06, Hir08, KZY09, KN04, LBG08, SKDO08, TBSM09, TCR+02, ZZL04]. decompositions [GPSP06, PBF07]. decoys [LZ05a, SRC03]. defect [ZMH+09]. defects [JT08]. Definition [EA06, LFSB03a, LFSB03b]. Definitive [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 [JHH01].
dehydrohalogenation [TT02]. deletion [SHE07]. delineate [MP03a].
delocalization [BY06, BI06, FVB08, FS02, Kar06, MGMM07a, MGMM07b, WMM03, WW03, WMW04, Van09]. deltorphin [OM04, YAÇ+C+02].
dEMON2K [GJK+06]. denatured [GB04]. dendrimeric [SCG04].
densities [GY08, GBJ03, HSWW00, KCK+08, LVM07, RLR+04, ZVZV06, Van02b].

Density [BP01, FC02, Han01, JCHS07, KWK+01, KWW+02, MSBS01, QZZZ03, QZL+04, VL00, WCW08, AB00, ABYM08, AEE+03, ASY01, Bac09, BP03, BMLV04, BB08, BAA07, CLP+05, CR+08, CFK08, CR+05, CR08, CSB08, CAG07, CPML08a, Cu04, CGSDST06, DVP+02, DVP+03, DF04, ECM+03, FCW06, FZL07, FDM00, FS04, GHLK+02, GLR02, Gri04, Gri06, GBB09, GHB04, HGMB04, HLS07, HNW07, HNW12, HN02, Hir08, Hol05, IIO2, ION07, IN08, IB04, ITN+05, IS07, JNV08, Jac09, JCA+02, JFG04, KGL07, KRM+02, KN04, KSS08, KU03, Kii00, KZW+05, Kri09a, KS01b, LRI+02, Lch06, LV08, LMB08, LMG05, LLS03, LWH06, LKT04, LF02, LLZL09, LLD+09, LZF+09, MP03a, MVW09, MS00, NK06, NTH09, NAT07, OKE+02, PSF+08, RB01, RK04, RLR04b, RDM+08, RR05, RZWS07, SH07, SZT08, SPT+03, SCF+09]. density [SLRC01, SSB07, SW06, TBG00, TST+08, TKN+08, TKH03, Van02b, VMA03, VBS09, VC04, VCK09, WR+06, WB07, WZY04, WMRW+01,
WL02, WCHW09, WM04, WCL05, WZXY07, WM01, XB08, XL02, XPW09, YTH01, YL09, YK08, YYW07, YLL+09, ZZL04, ZH08, Zho06, ZM03, vGGB00, Haf08, LWK08, MW00, XYN+06, GM01. \textit{density-functional} [HNWF07, HNWF12, LLS03, LWH06, TST+08, XB08, Haf08]. \textit{density/polarization} [YL09]. \textit{deoxyguanosine} [MM02]. \textit{deoxyribonucleoside} [PFR04b]. \textit{deoxyribose} [LBG08, SA07]. Dependence [ASS+02, MGLL03, BRLS08, BRLS12, BL00, KH06, NK06, SR09, TJM+03, VKCK09, ZP03, ZXY08, DvG00, DPM09, MG06]. \textit{dependencies} [FHF01]. \textit{dependency} [OKH02]. \textit{dependent} [Bac09, CFK08, FCW06, FCP+04a, Gog08, GS04, HNWF07, HNWF12, HS01, ION07, LDY+08, LDL09, LSW+01, MML02, MW09, MY08a, NTH09, OHNN00, PSF+08, TST+08, TKN+08, Wle08, WC08, YH07, ZH08, ZM03, vGGB00, PMM05]. \textit{depiction} [ZTS09]. \textit{deposit} [JG03]. \textit{deposition} [UNM+01]. \textit{deprotonated} [Mas04]. Derivation [EBD+01, JFG04, TT05, TTB01a, EBD+01, HZ06a, Tor02, Tot04]. \textit{derivative} [CNN07]. \textit{derivatives} [BT00, Bor03, BC06, CJK+02, COMR+04, DMC05, DSG06, FL08, GLRL02, IS03, PSF+08, PA05, QCK01, QCK02, RP09, SPGS08, SGPS09, Sch00, STC+08, TNS00]. \textit{derived} [GBJ03, HSWN01, Ish02, KSB09, KS06, KFNH08, MLJ03, svDS01, TBSM09, WMS06]. Deriving [RPMP03]. \textit{desaturation} [BBSS06]. \textit{descreening} [MTE04]. describe [DDBP09, IDMC09, MSH+06b, RLDI09, SBI08]. describing [CMaGLa04, HK08a, HK08b]. Description [ION07, MHT01, BUMCMRL00, BME05, CLWL09, CHRL09, Gri04, HGMB04, SM08a, VMA03]. \textit{descriptions} [SB08]. \textit{descriptor} [CDS09, RSS09, TCSM03, XYN+06, ZNL07]. \textit{descriptors} [AGMPRG+08, BAA07, DA01, EDAJ04, HM08, HMMS09, Jac09, LXW+09, GMGM07b, RUPH06, Tie09, TTB09, Wou00]. Design [AG03, KV00, BSP06a, BMTSC01, BLMS08, CRH+07, CMBC08, DB06, Dhw+07, Dhw+09, GHMP03, Ham07, HM06, HLTL09, HLM05, JGVF05, LBFSK07, LZ05b, LFS+07, MWE02, NHH05, FS09a, SPGS08, SRS07, SHM04, STCJ08, VGGM05, VZM+08, YFS07, ZZ08, ZL09a]. designed [GT03]. \textit{designing} [GDV03]. \textit{Desirability} [CMBC08]. \textit{Desirability-based} [CMBC08]. \textit{desolvation} [HMOG07, SVV+05]. Detailed [PB05, WRBV03]. details [GGB07a]. detecting [BHH+09]. Detection [WHH+06, BAL+01, CMCB08, OYH09]. \textit{determinant} [GS09]. \textit{determinants} [BCP03, Bou00]. \textit{Determination} [BLT03, CFR06, CR08, DLD+02, FSS00, Vas02, BL08, BR03, BCNs07, BdPRMIA00, CC09, Chi03, CAGR08, FAR02, GCCVB00, HP05, Mar03, MGLDS00, MM07, PC00, PFC03, PABK03, RI07, RTG00, SCF+09, TBSM09, vDSSvA04]. \textit{determinations} [YXL+09]. determine [DDVD09, KUB07, OO08, RIO8, YH06]. \textit{determined} [OYH05, TDH06]. determining [BY06, DV02, LR06, PHJ+08]. \textit{Deterministic} [LS05a]. detonation [JWB05]. \textit{detoxification} [ZWS+09]. developed [CRS05, KMH02, RG08]. Development
[ATMK03, BGJ01a, HHJ03, IS07, KSB+02, KOML08, KVL+04, LAT05, LK03, MSR04, MRC03, WWC+04, WWC+05, WS05b, XY+06, Yan04, BA08, COS01, CMGDAC+07, KLB03, NG04, BG03, IKYM09, SM08b].

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, FO08, FO04, FKS+09, GCCVB00, GKH05, GPS06, GKT04, HT05, HSWW00, HK07, HZ09, Hua09a, JPF+00, Kle02, Kle03, KTM02, NG04, BG03, IKYM09, SM08b, BA08, COS01, CMGDAC+07, KLB03, NG04, BG03, IKYM09, SM08b].

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].

diammineplatinum [DMN05].

diamond [EKO+01, JBGK08, ZMH+09].

dianionic [OSA06].

diatomic [ALKH04, FCW06, TLOG00, WWS07].

diatomics [Cul08].

diatropicity [CdML06].

diazonium [EL06, EL07].

diborane [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, HLN06, LZZC09, MML02, Vas02, ZFW08].

DIELS [Hir08].

DIESEL [ME06].

differ [SRK+00].

difference [ALC08, Bie04a, Bie04b, BF04, PMGP05, PZS04, 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 [VW04, BP09, Bie04a, CCCJ09, Rud05a, VW00, PK04].

difluoroethane [CSU00].

dihaloethanes [WFR08].

dihedral [FKZ09, HK08c, OFIK09, YL06].

dihydro [WJX+08].

dihydrololate [GGL09].

dihydrogen [Mck07b].

Dihydrophosphophosphophor [CDL06].

Dihydroxy [YXZ+04].

Dihydroxy [YXZ+04].

Dihydroxypyridine [HCMT04].

diiminobenzosemiquinonate [Bac09].

diiron [BB08].

diketiminate [GTC06].

diketone [RMP01].

dilute [HR05, Kr09b, XZ04].

dilution [DA01].

dimension [TSMNS01].

dimensional [BP01, Bie04a, CV08, DHW+08, LAR+03, LR06, MP03a, MVL06, RSS09, SHBD05, Wan09].

dimensionality [CDG09].

dimensions [AHK02].

dimer [CWY09, GYCZ04, Kr03, LZJ03, MPPK01, McD03, NK01, RRCA08, SB08, SG07b, YTH01, ZGXX06].

dimerization [HK07, JJK+00, WWK08].

dimers [BB1+09, FKRE08, GYMN07, LMGO+09].
dimethoxyethane [LCGA03]. dimethyl [GGGLL05, GWM+00, WLL+03, WJX+08].
dimethyl-2-iodobenzoylphosphonate [GWM+00]. dimethylethylenedioxy
[MTB09]. dimethylallylene [ZPL07]. dimethylamino [ZH08].
dimethylnitrous oxide [KZW+05]. dioxygen [BLO+02, SSW+07]. dipalmitoyl
[CEP07]. dipalmitoyl [CEP07]. diphosphates [PFR04b]. dipolar [RI08, San01].
dipole [DVP+02, EDW07, HN02, HK08a, HK08d, HK08b, KFZ03, MLA00].
dipole-quadrupole [HK08a, HK08b]. dipoles [DVRP+03]. Dirac
[HDBD04, PVdB00, TW03, Vis02]. Direct
[CBS+03, CAG07, JHH01, LW04a, TY03, WLLS04, WDX+02, YLZ08,
GLMV09, HP05, mJLZsLyL07, PC00, PFC03, SLL+04a, SHH07, STH+09,
UK04, WLL07a, WsLG+09, WLL+03, XLL+02, ZWL+05].
direct-particle-deletion [SHH07]. directly [SFRS01]. disaccharide
[FKJ+01]. disaccharides [SRB02]. DISCO [ZBS03]. DISCOtech [JFG04].
discover [LHJ+06]. discovery [HS07b, KV00]. discrete
[DXW08, MGLO03, QHL09, YL06, ZBS03]. discretization
[Bie04a, Bie04b, RP07b]. discriminant [ZHH09]. discriminants [FTLV01].
discriminating [yCkHmY08]. Discrimination [LDTS07, ZPL07].
discriminative [WHH+06]. discussion [CDGS09]. disilenes [TKS+01].
dismutase [PMM06]. dismutases [RJLR06]. Dispersion [COL+06,
RDM+08, CLZX09, GYM07, Grl06, JCHS07, KSS08, LB08, Weh08].
dispersive [BCF+09]. dissipative [YCXY03]. dissociation
[CJW+09, KWK+01, KWK+02, LS05b, TJM+03, WZZ+09]. dissociative
[ABYM08, KKJH08]. dissolution [SBG09b]. distal [IGNH03]. Distance
[MML02, RSS09, Ano05b, BL00, Cri04, IZA06, KvgH01, KH06, LI07, LHI09,
PYEA03, Sha05]. distance-dependence [BL00]. distance-limited
[Ano05b, Sha05]. distances [Var09]. Distorted [KS01b]. distortion
[LM009]. distributed
[ASWG07, DGRH02, FOK+04, ISO7, KMA+07, SKK+07, TYO+02, ZP03].
distribution [ACM+06, BBP09, CFS03, CV09, CMGDAC+07, JVV09,
KSO1a, KSO2a, LBT07, MZ05, MLG04, PP08b, SK09]. distributions
[AAE+03, BSP06b, Chi03, HLS07, LV08, MFB04, RLER05]. disulfide
[DWW+09, KF03, wQZsLyL02]. dithia-3,3-cyclohexane [FD03].
dithiane [FD03]. divalent [GS04]. diverse [AGMPRG+08, AVS09].
diversity [ZHH09]. divide [AKN07, vdVGDJ00, MLJ03]. divide-and-conquer
[AKN07, MLJ03]. dizincocene [GXK09]. DL_POLY [KSY+00]. DMPC
[HNL08]. DMS [RAGL09a, RAGL09b]. DMS-0H [RAGL09a]. DMSO
DNA [AB08, AZM03, BCP03, DLW06, DLWV07, 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].
DNA-base [AB08, AZM03, BCP03, DLW06, DLWV07, 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].
dynamics [Maz01, MVL+05, MO09, MH08b, MCM04, MST+08, MS01, NK01, NBJ04, NYK+09, OO04, OO06, OR05, ON07, PMGL03, PRKP05, PMB04, PBW05, Pin01, Pin03, PYS08, PHH+08, PHRR08, PB02, PNG08, QNF09, RRZ08, RMM03, RG08, SH09, SB08, SBL09, LMA00, KMLZ07, JHZ09, KMH02, KˇSB09, KM00, KM07, KSY+00, KAK+09, KZRO03, Kol04, KV04, KPR04, Kri08, Kri09b, Kr603, LLM08, LG06, LGK+07, LYY+09, LR03b, Loe03, LMIF06, LM03, LPB03, MB00, MFB04, MN02, MABM09, MBC08, MCR08, MDA08, MOP+07].

dynamics-quantum [ZSK07].
dynamics/order [MO09].
dynamo [FAB+00].
Dyson [SVT09].

Edited [Sta00]. Editor [JW12, WM12, vLBBR12, Lip00]. editor-in-chief [Lip00]. Editorial [Bro05]. Editors [BFS07, FA01b, FSB09]. educating [BS01]. Effect [CXZ+09, CN05, CEP07, KGL07, Mue01, WME04, BB08, CP00, CP01, CGB+09, CSB08, CKT+08, DMJ05, GT03, HK08a, HK08b, KT08, KMM07, KCL00, Kri08, Lee09, LL01, LCA03, Mas04, MZL08, PCS04, RY09, RR05, SO05, SPDS01, SCG04, SDL07, VM07, WM06, WDX+02, XWL+09, ZY01, ZZR+07, ZWPR+04, CPDZ08, HFS+07, JD09, WMW03, WSC09, vE01].
Effective [OCB02, SBLK01, VBG+00, BCF+09, CR09a, DPT03, HMW03, HSWW00, LFK05, MML02, NGBT03, NG04, RPMP03, SG07b, VB02].

effectively [SMGE08]. Effects [DXW08, KKH+07, RLP08, WX08, AD00, ASS+02, BA03, BA04a, BA04b, BPC01, BE07, BDW00, BBI+09, CC07, CKF01, CDPL09, Don01, Dra00, ECA06, FGR07, FHF+01, GMM08, GVATG03, GM04, GGLR00, GKS04, HRR05, IC08, JJK+00, JWB05, KSK00, LS08b, LR03b, Loe03, LFR+04, MDA08, PBF09, PSF+08, PWFS01, RRC08, SF07, SL09, SMAV00, SURG06, SM06, SN06, SRB06, VDM06, WMGK07, WD04, Wib04, XYN+06, YXZ+04, YH09, Z04, ZWS+02, CM09].
efficacy [KSM05]. Efficiency [IO08, MKGA06, RLR04a, YA+02, CN03, FSB09, GF08, KK08a, LJD04, LJ05, LK04, PSM05, SM08b, SM03, SE08, vLBBR12]. Efficient [AT02, BP00, BB05, CS01, DMZT08, EA08, FL08, FKZ09, GHH07, GB04, HMW03, HTHG08, KMA+07, KCL00, Nil09, OD09, Oos09, SAT04, SSM08, TP01b, WM12, YZ04, AMI00, BL09, BP02, BPR01, C00, CG06, CI05, CY09, CY13, DBS08, FG02, GJL+08, JJB00, JJB02, KM00, LSO04,
LCKL05, PRSMM02, RKA+09, SAM06, SSMW09, TS05, Tot04, WW03, YXL+09, vLBBR12, FS09, FS00a. efficiently [IGL07, LR06]. eigenvalue [SSL02].
eight [CWW+05]. elastic [AJ03, BED02]. Electric [LTV08, SF07, WMS06, ÁCD+03, BSOB05, CM09, Kar06, LST08, Mar03, OBBS05].
electrical [KCL00].
eletric [CWW06].
electric [AJ03, BED02]. Electric [LTV08, SF07, WMS06, ACD+03, BSOB05, CM09, Kar06, LST08, Mar03, OBBS05].
electrochemical [Bie04a, Bie04b, Rud05c].
electrocyclization [ZGZX07].
electrolyte [CCCJ09, YSJ09].
electron-correlation [YH09]. electron-pair [FS04]. electron-repulsion [Kri09a].
electron-sharing [BRS07].
electron-transfer [QZZZ03].
electron/four [GYMN07].
electronnegativities [dSGCG00].
electronnegativity [ALC08, BCNs07, JVVK09, VK06].
Electronic [CWW07, DHH+03, FLK+07, GGGGL05, Hua09a, IIE02, KHY00, KMM07, KGD06, LPP06, LTF+07, OS08, QB05, RPNJ07, SCP08, Wu06, WWS07, XZ05, AJ03, AEE+03, Ama02a, AZS+04, AGSFA+05, ASS+02, Bac09, BBG+04, CMaGL+04, CZFH07, CN05, CNN07, CAG07, CRS03, CSV+07, CTF08, DD00, FL08, GJL+08, GBL+05, GM04, HMM09, HZ09, Hua09b, Kar01, KRM+02, KJP+07, KIFK07, KWK+00, Kri09a, KPZK06, LW08, LWS07, LWZ09, LFR07, LB08, LDL+09, LMRFV+09, MKGA06, MM02, NYH02, PP08b, PMC+08, QC01, QCK02, RRC08, RS05, SS03, SBL05, TD08, TT01, TD06, TDK07, WMRW+01, WLX+05, WL00, YXZ+04, YFR05, YS00, ZZZ+07, ZZZ+08, ZYYF09, ZXX08, ZL05, ZL07, ZL09b, ZM03, SMKM00].
electrons [HIM07, Pog03, WJ00].
electroosmotic [YS09].
electrophilicity [RUPH06].
electrophoresis [WWL+09].
Electrostat [CCT+03, GYMN07, PK05, PML03, RLER04b, SG07b, ABWT09, BCNs07, CPUGD09, CHMI05, DWN01, FOL+04, GY06, GPK05, GJ03, KFZ03, KLH+04, KCK+08, MMPK01, PMB04, PP08b, RL08, SMAd00, SFS05, VGDS08, VC04, WCK00, YH06].
electrostatics [HS01, MLJ03, RS03, STS02, VVVB02, WMS06, ZFW08].
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, CFS03, FSS00, PC05, PC07]. ELI [BBW+08]. ELIA [BBW+08]. elimination
[Adc04, CFD03, GLD08, GS08, KUB07, Mui05, PSDM00, YFS07].

**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, HRBKB03, JCHS07, KK08b, LR03a, LLM09, MB00, RKH03, ZNLL07, VBGL+00]. **employing** [MHT01, THHN01]. **empty** [CZA03]. **enantiomerization** [Qua07].

**Encapsulated** [CEP07, GGLR00].

**Encyclopedia** [vRS98, Lip00].

**End** [Adc04, GLD08, KUB07, PSDM00, YFS07]. **endohedral** [KSN01]. **endoperoxide** [BLO+02, CG08].

**Energetic** [DRAS04, DRAS05, JW12, RP09, BCP03, ECM+03, JD09, KCK+08, PBF07, SLHW09].

**Energetics** [KRLD09, AHGK09, DBGV07, Hua09b, ILKR09, LD05a, MFB04, MLL+08b, NHH05, PK05, PSF+08, RSSKB03, RSE07, RSN+02, RM00, SZT08, STSF02, SYC03, SA07, SLRC01, TKS+01, UBDPJ04, Var09, VC04, WCK00, WLX+05, WS05b, WW04, XLT07, ZM09, ZW09, ZM03, vGG00].

**Energies** [CBH+03, HFHL06, IN08, KLS02, MSF+08, NK06, SS07, WM12, dSR08, AMR04, A03, ABA04, AE06, AM06b, ABBC01a, ABBC01b, AGSFAL05, BM07, BCI05, Ber03, BL05, Bl04, Bo01, BRL08, BRLS12, BACJCT01, BF07, BLB09, CC09, CN03, CCB04, CY09, CY13, CJS+09, Chi03, yCkHmY08, CV09, CMGDAC+07, CA04, COL+06, DLD+02, DLRZ09, DMV05, DKL01, EGSG00, FMS09, FK07a, FKJ+01, FZL+06, GLZ02, GMA04, GLMV09, GAdGM08, GG09, GC04, GS02, GS03, GPSP06, GB02, GWS+02, HKMS01, HP01, HR08, HMOG07, IGHN03, ILKR09, IGL07, IPN06, IPN07, Jac09, JMD+02, KGN07, KN04, KKC05, KUB07, KB09, Kob03, KC01b, Kri09a, Lab08, LR03a, LMK01, LF04, LFZS04, LJO04, LB08, LKW04, L09, MG06, MCF05, MAF+07, Maz08, MH09, MGJAARC00, MGL003, MRS+07, Nak02, NKIS02, NA06]. **energy** [O09, OF08, ONNH00, OKH+02, OV3, Oos09, PSC+01, PMGL03, PK04, PAT+09, PMGP05, Q0a1, RP07a, Raa00b, Rap06, RSE07, RRCA08, RWBH09, RHL09, SOOF05, SPDS01, SKGS00, SPL+02, Sch03, SMGEO8, Sen06, SDEC03, SSM08, SY09, SG07b, SSMW09, SMD02, SJW09, SSBE06, TJE03, TGGP+00, TCR+02, UTH+03, VE09, VM02, Vya01, WL02, W04, Wh08, 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 BS₄⁺₀₁ EMP07 OO06 SM08b SM03] ensembles [GLD08 Ik04] ensure [FKFG08] entero virus [KCL06] Enthalpies [EB04 WC04 BE06 LS05b RM00 TTTBM09 VGGMM05] enthalpy [OVMV04] entire [ZAT07] entropic [CBC⁺₀₈ FGR07] entropy [DHF⁺₀₅ HDF⁺₀₇ HTKG08 KKH⁺₀₇ LM03 RK05 Ruv07 STSF02 WG02] enumeration [AL01] Envelope [BHH⁺₀₉ CV09] Enveloping [BHH⁺₀₉ CV09] Envelope [BA04a BRLS12 CY13 FS00a HHW00 BH03 BF04 BF07 BRS00 BRS01 FS00b Ho05 HBW00 HBW01 SAT004 TW03 Vas02 Vis02 Zho06] equations [AMR04 ABWT09 BH03 BF04 BF07 BRS00 BRS01 FS00b Ho05 HBW00 HBW01 SAT004 TW03 Vas02 Vis02 Zho06] equation [AMR04 ABWT09 BH03 BF04 BF07 BRS00 BRS01 FS00b Ho05 HBW00 HBW01 SAT004 TW03 Vas02 Vis02 Zho06] equations [AMR04 ABWT09 BH03 BF04 BF07 BRS00 BRS01 FS00b Ho05 HBW00 HBW01 SAT004 TW03 Vas02 Vis02 Zho06] error [IO08 KMA⁺₀₇ Kob03 Mas04 MDI04 RS05 Rud05a Rud05b Rud05c] error-ranked [TBSM09] errors [CS03] error-ranked [TBSM09] errors [CS03] erythronic [vDSSvA04] ESFF [SYY⁺₀₃] Essay [BHTCG07 FK07b GR07 Kuo07 MGCA07 Nye07 Shu07 Sim07 Tru07] established [SB01] ester [TH02] esters [POJ01] estimate [KC01b YZ04] estimated [ZMZ09] estimates [GC04 HT05 MDI05 SY09] estimating [HDF⁺₀₇] Estimation [HDF⁺₀₅ ZW09 CV09 DDVD09 HTLTP09 KC01b PYEA03 Lab08] estimators [GZL02] estrogen [FKU⁺₀₅ KBK⁺₀₁] ethane [DGD⁺₀₅] ethanes [WyLG⁺₀₉] ethene [Ang09] ether [GRL02 WD04 WLL⁺₀₃ YLW⁺₀₈] ethers [ACL03 LCA03 LCGA03 LCA03 ZWY⁺₀₉] ethyl [KKH⁺₀₇] Ethylene [TBG00 BSJ01 Hri08 NTH00 SBB02] Euclidean [RRS09] EUDOC [PPXP01] Euler [SG01] evaluate [GGB07a GGB07b LF04 OSH03 TSSGS07] evaluated [ABB01a ABBC01b Bof01] evaluating [FO08 Con02] Evaluation [BMLV04 DR07 KSM05 NMAT01 OYH09 VKP⁺₀₈ YSJ09]
Ano05b, AGSFAL05, CGG06, CAG07, JSR+07, DBS08, ESP04, FMAMVK06, FKZ09, GGA00, HMWC03, JSHG07, KJVW08, 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]. evaluate [SF05]. Evans [SRK+00].

EVEBAT [CZA03]. Even [CVVB04, CC07, VVBV02]. Even-tempered [CVVB04]. evidence [BLO+02, IO08, SFR07].

Evolution [SPL+02, Der09, Mck07a].

exact [GC02, GHMP03, DLSVY00, TRS02]. examination [CZA03, LJKL08, QNF09, WL04, AB˚A04]. example [AS00, JHPRSM+05, MGLL03]. 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, XZ04]. Excited [CHA+07, HFS+07, Ang09, FCW06, FDSA00, HNWF07, HNWF12, IR03, LWX07, LDL+09, MW09, NBTN04a, NBTN04b, NTH09, PO03, PSS+04, SBI08, SMKM00, TY03, TKN+08, WLZ+07, 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, WBRS03, ZFL+05]. expansions [Bou01, DWNB01, GC02, JSHG07, RLER04b, SG01]. experiment [BE09, GB303, LS05b, Mat03]. experimental [BE06, JARM02, LEK07]. experimentally [KBN02, TDH06]. experiments [CVR08, HP05, OD09, PC00, PFC03, SL04]. Explicit [EC06, PPYS08, RI07, AL01, DMJV05, FC06, HM02, JZD+09, KIFK07, KIM+09, LSO04, PK05, RKA+09, WB04a, WB04b, WB05, ZGFL01]. explicit/implicit [LS004]. exploiting [JSHG07]. exploration [CSJ+01, HLB09, LXW+09, LM009]. exploratory [PGH+04]. explore [ILKR09]. Explorer [SHBD05]. Exploring [BL05, HP00, HXLS09, KFO8, Sch03, Tie09, SPL+02]. exponent [WTKM06]. exponential [Rud05a, Rud05b, Rud05c]. exponentially [Bie04a]. exponents [MY08b]. exposure [MML02]. expression [dGWH01]. expressions [TNS00]. Extended [LMH+09, TVL+03, Bie04b, Ciu04, DXW08, KUB07, QNF09, SS00, ST01].

Extending [GCD04, MFB04]. extensible [SY+03, GBL+05]. Extension [CR09b, FBL08, 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 [MO09, MC06, PSC+01, PFJ+03]. extremal [ZZ08]. extremely [GFS05].

Eyring [Nye07].

F
[CRC+08, FO04, Gog08, HYA02, HZ09, Hua09a, IV04, KS05a, KBL08, Mar03, RB01, STC+08, UTT+04, WLLS04, WLL07a, XLL+02, ZY01, ZLLS06b, ZL09b, HK07, KS05a, RFSS06, SOOF05, Sha02, WDWS06, YWHZ03].

facility [SWZS04]. factor [LMCD09, WL00, XSHC06]. factorization [EC06]. factors [AST06, SBH02, TP01b]. FACTS [HC08]. family [CFS+09, DMC05, NAT07, WTKM06]. FapydG [SHD+08]. farnesyl [SFR07].

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

field [SDCG02, SSS+09, SYY+03, SHK+05, SP05, SK05, TAS07, TTB01a, VSW+03, VCM01, VTT+08, WK01, WWC+04, WWC+05, ZWZ+06, WMS06, Wli01a, Wli01b, XL07, YCXY03, ZWC+09, vDSSvA04].

field-based [DMLI05]. field-derived [WMS06]. field-induced [CGB03].

fields [ABA04, Car02, EBD+01, HRBKB03, LLM08, Mac04, MFB04, OSHS03, PK04, PB02, RP07a, RL04b, 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,
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, RJK03, SDL+09, SD+0G01, SAS05, SDCG02, SF05, SSS+09]. force
[SY+03, SHK+05, SP05, SMM+08, SK05, TAS07, TTBM09, WVC+04, WVC+05, WZW+06, WJ01a, WJ01b,
XL07]. Force-field [CLP09, OBT09, SO09, HGBM04, 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, RAGL09a, RAGL09b, BE06, BMTR08, CS03, EB04,
HAA03, JWB05, KLE02, LLAO11, LYZ+08, NEE03, RCJ02a, RM00, TT08,
TTBM09, WC04, WX09, ZW09, DOEML01, JKM08]. formed
[LL02, LSW+01]. formic [Pac06]. forming [PP08a]. forms [SPT07].
formulas [Ish02, Tor02]. formulation [BF07, Cul08, PK05]. formyl
[GS09, HJCP01, FFC03]. formylglycinamide [HRKB03]. forward
[KM07, SJ+04]. Four
[SH02, FJ08, GPS06, 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 [MGL03, SM08b]. fragilis [SDM02].
Fragment [DH+09, CFK08, DPM09, FOK+04, FKL+06, FII+07, FKU+05,
FKU+06, FKM+07, IJK09, KIFK07, MLG04, ML08a, NYK+09, NGTB03,
NG04, OO08, SG07b, ZM09, KIM+09]. Fragment-based [DH+09].
fragmental [CS+03]. fragmentation [Gor01]. fragments
[AM09, DWNB01, DPPR05, KS01a, LV08, NG04, PBF07]. Framework
[JGVF05, CR08, EA08, FS04, TAS07, Tie09]. Framework-based [JGVF05].
Franck [Ama02a, LMCD09, TP01b]. Free
[DLR09, GS03, JMD+02, MH09, PMG03, YX+07, AM06b, BWE05,
BL+06, BCI05, BLo04, CNO3, CM09, CY09, CY13, CH03, CV09, CCK01,
CMG01]. CO+07, CG05, COL+06, DMJ05, FSM09, GZL02, GMA04,
GMV09, GG09, GC04, GS02, Gra07, GWS+02, HMK01, HR08, HMOG07,
ILK09, IGL07, JZD+09, KDG+09, KAS+07, 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, RE07, RWBH09, SOOF05, SAM06, SKGS00, STSF02, SBL05,
SSM08, SY09, UBDPJ04, UTH+05, VE09, VGDSU08, VM02, WHF08, XLT07, YZ04, ZMZ09. free-base [SBL05]. Free-energy
[JMD+02, AM06b, CY09, GMA04, ONHN00, RWBH09, SKGS00].
Free-energy-driven [MH09]. freedom [DHF+05, MZL08].
freeze [BME05]. freeze-and-cut [BME05].
frequencies [BRV+07, Han01, KBN02, LMB08, PZWG+04, WM04, ZWPR+04].
frequency [DF06, DR09, MY08a, VSW+03, YH07]. frequency-dependent
[MY08a, YH07]. friction [JS07a]. frozen [AEE+03, GWS+02, JNV08].
frozen-density [JNV08]. fructose [MRS+07]. fuel [CCCJ09].
Fujitsu [KSY+00]. Fukui [DVP+02, FS04, TSSGS07]. fulfillment [RLER07].
Full [PRSMV08, GD09, IR03, KGD06, RS08, ZCZ03].
full-atom [RS08]. fullerene [CHRL09, CTFC08, GYCZ04, GXK09, Kan07].
fullerene-dizincocene [GXK09]. fullerences [GZ07, GM01]. Fully
[GWM+00, XZZ04, WTKM06]. function
[Bac04, BS05, BdPRMAI00, CFS+09, Che01, yCkHmY08, CPUGD09, Con02,
DMZT08, DP03, FSS00, GCB03, GS09, GdAcV+07, GP01, HMWC03,
HZ06a, HZ06b, ILB03, ILKR09, Ish04, KK60c, Ki00, KFD06, LR03a, LHI09,
LB07, MP03a, MML02, MY08b, Nak07, NIK02, PP08b, PA05, PAS07,
SFC04, SJW09, TLKT00, TV03, TJE03, TT05, TSSGS07, VVS07, YLL+09].
functional [AAP00, AB00, ABYM08, ASY01, Bac09, BP01, BE09, CLP+05,
CFK08, CR05, CR08, CB08, CPML08a, Cu04, DVRP+03, ECM+03, EL09,
FCW06, FZL09, FG02, GHLK02, GM01, GLRL02, Gri04, Gri06, GBBH09,
Haf08, Han01, HNW07, HNW12, Hol05, ION07, IB04, ITN+05, IS07,
JFG04, JCHS07, KGL07, KSS08, KWK+01, KWK+02, KZV+05, Kri09a,
LR01+02, IWK08, LMB08, LMG05, LSL03, LW06, LKT04, LF02, LLZL09,
LD07+09, LZF+09, MW09, MSB01, MW00, NTH09, NAT07, OKE+02,
PSF+08, PU09, PDS01, QZ03, QZL+04, RB01, RK04, RDM+08, RR05,
RZWS07, SH07, SHT08, SPT+03, SPT07, SRLC01, SSB07, SW06, TBC00,
TST+08, TK04, TKH03, Van02b, VMA03, VL00, VBS09, WR+06,
WB07, WZY04, WMRW+01, WL02, WCM08, WCHW09, WM04, WSC09,
WCL05, WZXY07, WM01, XYN+06, XB08, XWC09, XL02].
functional [XPW09, YYW07, YLL+09, ZZL04, ZH08, Zho06, ZM03, vGGB00].
functional/continuum [LRI+02].
functionals [BP03, DF04, Han01, ION07, JPCA08, KR+02, KS01b, PJPRMI07, SCF+09, WL04, YTH01].
functions [AE06, Bac07, Bou00, CGB03, CGdST06, DVRP+02, GFS05,
GLD08, GS07, GB03, IT03, LLC06, MY08a, NU02, OFB08, PFB05,
RL09, Ruv07, SS00, TS05, TD06, WG02, YH06, ZM03]. Fundamental
[LMB08].
funi [LPP06]. funnel [HEP+02]. furfural [COM+04].
Further [GPK05]. fusion [CRGN07]. fuzzy [ALTB06, EKB02a, RLA01].
FVII [PDP02].

G [AGI+07, Kr03, XWC09]. G** [Wib04]. G-protein [XWC09]. G.
[CS05, Sim07]. G2 [RY09, ZKZ+07]. GA [HSMT04, HSMT04, LL+08].
GA-MLR [HSMT04, LL+08]. gadolinium [AB00]. gain [HP05]. gains
galabiose [RSSKB03]. galactose [RSSKB03]. GAMESS
[UKNS01, UKN04]. gamma [Ish04]. gap [KUB07]. gap-free [KUB07]. Gas
[BAL+01, POJ01, CPJ00, CPJ01, DR09, EGSG00, JJK+00, JHZ09, KSB+02,
KT08, KKH+07, LRI+09, Lee09, LZA02, LB05, LXS+08, MFB04, Mas01a,
Mas01b, MM02, Pan07, PV07, wQZsLyZ02, RRS06, ROG00, SMGE08,
STSF02, SMKM00, SK05, TDH06, UCT+03, UNM+01, WD04, XKKL03,
XKG+05, YQHH09]. Gas-phase [BAL+01, POJ01, JHZ09, KKH+07, Lee09,
MFB04, wQZsLyZ02, TDH06, UCT+03, XKKL03, YQHH09].
Gaseous [WDWS06, PG01].
Gaseous [WDWS06, PG01].
gases [SRB06].
gauge [Ish03]. gauge-including [Ish03].
Gauss [DBS08]. Gaussian
[TdMSD+08, CMJ08, Duk01, EDW07, GC02, HdMdS05, HdS06, HD06, IO08,
Leh06, Lu09, MV06, MY08a, RC04, TW03, WTKM06, YJF06].
Gaussian-2 [RC04].
Gaussian-type [Leh06, MY08a, TW03].
GAUSSIAN94 [Kli01].
GB [GC04, WHF08, GWS+02, YJF06].
GBR [FPG+06].
GDDI [FOK+04].
Ge [WDX06, CJS+03, LLXS02].
GeD [WDX+02].
GeH [LLXS02].
gemcitabine [PFR04a].
geminals [TT05].
geminal [TT05].
general [AM07, BR01, DG+08, EBD+01, JMB07, KSU03, KBT03, NUH02, RG08,
SAM06, TZX01b, TXZ01a, WWC+04, WWC+05, XYN+06, BRS07, EA08,
FLGW00].
generalizable [KYT+08].
Generalized [ADM+06, ILB03, AB08, BC06, Bud07, CPJ00, CF06, Cui08,
DLG00, FOL+04, FL08, FC06, GZL02, ION07, Lab08, LFSB03a, LFSB03b,
MTE04, MCM04, OCB02, SHH07, Tot04, XL02, YH07, YJF06, ZGFL01, dGWH01,
BPCD07, FOK+04].
generate [BWI+02, CA07a, BAH+02].
generated [Kri09a, LAR+03].
generating [AMR04, CA04].
Generation [RLER07, BSO05, BAH+02, EL07, EKB02a,
JB00, JJB02, KSB+02, LS08b, MM03, PVdJB00, PAK03, YJF06].
generator [Fan01, HDBD04, LN01, VW00].
generic [yChYm08, Yan04].
Genetic [LSY02, MM07, YL06, BMTSC01, CKMC04, HHJ03, HWBD03,
HMSM06, KOFF09, LJ505, SPT07, SBH02, TP01a, WK01].
Geometric [CSRT04, ZZTS09, Est07, LDL+09, RSN+02, ZXY08].
geometrical [GRCD01, KLE03, MLL+08b, PB+07, SCF+09, GCD04]. geometries
[BB08, Han01, IZA06, JCHS07, KKY01, KJP+07, WB07, Wib04].
Geometry [Bud07, LHP01, RK04, VMF+03, BP00, Bie04a, BM00, Cri04, GPS06,
HHBH00, IZA06, KKG+09, KHF+09, Kle03, LJ04, MBP09, MW00, PO03,
Pul05, RON02, SCP08, WPS02, ZS+07].
GEPOL [PTC01].
Germanium [LLXS02].
GFP [HFS+07, NINAT+07].
GGA [DDBP09, Gri06, RLDI09].
GGA-type [Gri06].
GIAO [FO04].
Gibbs
e [EGSG00, HR08, IGL07, Lu09, SM08b].
Gilbert [GR07].
Gillespie [RMP01].
give [JJK+00]. glasses [NA06].
Global
[CZB07, FTLV01, JHZ09, CS02, CMBC08, LS05a, RUPH06, SE08, TSSG07,
TSSG08, WS02a, WG02, UKN04].
Globally [PAS08, SPT07].
Glu441
[PCS04].
glcans [CMD+04].
glutamate [FTLV01].
glutamic [ZZY07].
glutamine [WC08].
Gly [PC00, VKP+08].
GLYCAM06
[KYT+08, SDL+09].
glycinamide [LB05].
glycine
[BA03, BA04a, BA04b, GAIMVB01, GSB09, GKTS04, KAS+07, LB05, LSW+01, MOP+07, PG01, ROG00, ZW09]. glycol [Pin01, RR05].
glycol-lesioned [Pin01]. glycosidase [BMTFR08]. glycosidase-inhibitor [BMTFR08]. glycosidase-substrate [BMTFR08]. glycosidic
[SO09, SDL+09]. glycy [KOML08]. going [CC01], gold [BR04, CZ05].
gold-capped [CZ05]. GoIP [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, HXLS09, MBC08, SBJ08, VSK+04, VTT+08, WWL+09].
graining [CA07a, EBA07]. grand [EMP07]. GRAPE [Höf05].
graphe [CLX09, MGMM07a, Pog03]. Graphical
[LD05b, DPDG05, JKI08, KMH02, KBT03, LW04b, LZX06, Pra01, YNW05, hYDN+08]. graphically [GS09]. graphics [FEV+09, SP07+09, Yas08].
grape [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].
GROMACS [KV+07, LSG06, VLH+05]. GROMOS
[CLL09, CHB+05, LH05, OVMV04, SHK+05]. GROMOS05 [CHB+05].
GROMOS96 [SDG01]. grove [BCP03]. grossular [ZWT+08]. Ground
[HM01, PO03, PSS+04, BBI+09, CWY09, FCW06, FDSA00, IR03, Kri09a, LMK01, ZOJ+06]. Ground- [PSS+04]. Ground-state
[HM01, Kri09a, LMK01, ZOJ+06]. group [ATBS04, CQ04, DVR0+03, EIL07, EBO4, JWB05, JGH00, KBT03, LW07, MBM+00, MA05, RCJ02a, RZWS07, RKH03, SGP09, SN00, TD06, dSGCC00]. groups
[BE09, EBO4, FJ08, VAO2a, WSC09]. growing [Qua07]. grown [WHH+06]. Growth
[TDK07, HMK02]. Grubbs [YX+07]. Grubbs- [YX+07]. GS
[MH09]. GS- [MH09]. GTO [CG03, RLRE01]. guanine
[EL07, GWL07, HWWG08, JMO7a, KKCM04, MSBS01, MHS05, SMKM00]. guanine- [MHS05]. guanine-cytosine [KKCM04]. guess [Qua07]. guest
[LMWW04, OS09]. GUI [JKII08, SD09]. Guide
[SH08, Woo01, You11, Bie09]. guideline [MWE02].

H [AGI+07, BAL+01, BPC01, BL00, CP00, CS01, DRAS04, GPSP06, HYA02, IN08, IS03, LDMR01, LMK01, LLXS02, LW04a, LYZ+08, LMO09, Mas01a, Mas01b, MGLL03, SLL+04b, TNY05, UTC+03, WDX06, XDS06a, ZZ07, ZZZ+06, dRLM00, CPDZH08, CFW+09, CGB03, DLD+02, Don08, Ed0VR+03, Gog08, HK07, IT06, LC07, LDC+07, LLXS02, LB05, LN01, LLL07, LS05b, LMO09, MR02, McD08, MY08a, NL08, OO04, PGR0NG03,
PRSMM03, PV07, RFSS06, RWBH09, SOOF05, SEKS09, SLL+04a, WDS06, WTKM06, Wei08, Wil01b, WDX+02, YTY07, ZY01. **H-bonded**
[LB05, McD08, NL08]. **H-NMR** [AG+07, H5N1 [DLRZ09]]. **Hairpin** [ZHH09, CJW+09, LHI09]. **Hairpins** [IGNH03, Der00]. **Half** [FMAMVK06, PS03, PMM06]. **Half-numerical** [FMAMVK06]. **Half-reaction** [PS03, PMM06]. **Halide** [RC04, CW02]. **Halides** [AB00, LYK+04, LSY02, ZJM+07]. **Hall** [SPGS08]. **Hallah** [TBGRJ04]. **Halothane** [TZX01b, TZX01a]. **Hamiltonian** [FGR07, FBLO08, MR02, SAM06, ZWPR+04]. **Hamiltonians** [CV09]. **Hand** [DFGB09]. **Handle** [GCD04, GM04]. **Hansen** [BBG+04]. **Haptic** [MR09]. **Hard** [TGGP+00, ZHMW09]. **Hardness** [PRS04, TSSGS07, TSSSG08]. **Hardware** [ATMK03]. **Harmonic** [CLP+05, Ish02, TFN04]. **Harris** [Cul04]. **Hartree** [WMW04, AKN07, Biot00, Cul04, DDD00, GAdGM08, MS00, MBWP03, PFJ+03, RRS07, WMW03, Wei08, YH07]. **HASXH** [LS08a]. **Having** [WJ00]. **Haystack** [BS01]. **HBCC** [BAL+01]. **HBOP** [OYH09]. **HCO** [JPF+00, dRLMS00]. **HCO-L-SER-NH** [JPF+00]. **HDMR** [LRWG03, LAR+03, LSHR04]. **Head** [HSWN01]. **Heart** [TKH07]. **Heartland** [Sha07]. **Heat** [dOMSL01]. **Heats** [CS03, JWB05, RCJ02a, WX09, LLA01c]. **Heavier** [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** [IGNH03]. **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, YAC+02]. **Herbicidal** [XYN+06]. **hERG** [MCR08]. **Hess** [YH09]. **Hessian** [KK01a, NKS02]. **Hessian-free** [KK01a]. **Hessians** [ASWG07, Chu07]. **Heteroaromatic** [LLM09]. **Heterobimetallic** [RD00]. **Heterochiral** [ZOJ+06]. **Heterocycles** [FSS00, MGMM07b]. **Heterofluorenes** [CZFH07]. **Heterogeneity** [HS01, ZSC05]. **Heterogeneous** [FCK+08, ZCS04]. **Heterohelicenes** [LC09]. **Heterolevel** [EA08]. **Heteropentalenes** [CDL06]. **Heteropolymers** [SBJ08]. **Heuristic** [DMC05, DLHC06, CAGR08, IZA06]. **Heusler** [GD09, KG06]. **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, GKT04, PMPGP05, WW03]. **HF/6** [FKJ+01].
HF/6-31G* [FKJ+01], HF/DFT [BRLS12, BRLS08], HF/MP2 [GKT+04], HF/HF [JHPRSM+05], Hg [GPS+06, BBI+09, WTKM06]. HH [CMaGL+04], HI [KKJH08], Hibert [Hb09]. hidden
[FWH+07, HL+05, RP07a]. Hierarchic [RRS07]. Hierarchical
[LMH+09, CWV+05, DJB02, FOK+04, LLC09, UIHN09]. High
[BB08, GA+08, LA+05, AZ03, BACJCT01, CCW02, CN05, DPT03, GL04a, GY08, HGMB04, JB00, JJB02, KKW+00, KF08, LR06, Mck07a, Mck07b, MTB09, RP07c, RLER07, RSS09, SSS+09, WMRW+01, WS05b, XK08, UT+02]. High-dimensional [LR+03, LR06, SSS09].
high-latency [KVF+07]. high-level [WS05b]. high-resolution [GK+04, CWW+05, DJB02, FOK+04, LCC09, UIHN09]. High
[BB08, GA+08, LA+05, SSS+09]. High-dimensional [LR+03, LR06, SSS09].
high-valent [AZ03, CN05]. higher [BdPRMAI00, LMGR05].
highly [ZFW08, BLL+06, CMD+04, GZL02, HB09, HNB01, Han01, ION07, JPCA08, JIK09, KRM+02, KN04, LSO04, LW02, LS05b, MBM+00, MSH+06a, PDS01, RMD+08, Sza08, TTHN01, TFN04, WWL+09, XL08, ZZL04]. Hybridized [SJ+04]. hydrates [GXX09, Kan07]. hydrate [ME+02].
hydration-parametrized [RP03]. hydrazines [BL01]. hydrazones [Lu09]. Hydride [GVAT03, JIH01, LLX02]. hydrides
[KS01b, SRB06, sSGCG00]. hydridotris [HT05]. hydridans [HKHN08].
hydrocarbon [CS01, KFD06, LC06, Wan09, WEE01]. hydrocarbons
Hydrodynamic [BZP09]. Hydrogen [AG00, Kle03, RP04, XZ04, ZX04, AD00, AST06, BM07, BUMCMRL00, BL06, CUS00, CUSS03, CPDZH08, CVVB04, CCK01, CPDL09, DR07, EFQD09, GAIMVB01, HDMS05, HS06, HRG07, HIA03, HT03, HA04, IO08, JP09, mJlZsLyL07, Kle02, LC07, LDC07, LW04a, LDL09, Mck07a, MH08a, NHH05, OO08, PG01, Pac06, PGG06, Pog06, Rao00a, RM07, SPT03, SJW09, TGLL07, WLLS04, WZZ09, WJ00, ZKZ07].

Hydrogen-abstraction [WLLS04].

Hydrogen-bond [RM07, SPT03].

Hydrogen-bonded [CPDZH08, LDL09, MH08a, ZH08, vEMK01, vE01].

Hydrogen-bonding [AG00, ZW09, Yos02].

Hydrogenase [TDH06].

Hydrolases [OBT09].

Hydrolyses [DWS09, LYK04].

Hydrolysis [WOC03, DLR08, MBL00, RP04, TH02, WXX03].

Hydroperoxy [BL06].

Hydrophilicity [DLHC06].

Hydrophobic [MBH02, CJDK09, HJCP01, SDL07].

Hydroxide [CBS03].

Hydroxy [CUS00].

Hydroxyacetone [WXX03].

Hydroxyaromatic [BLO02].

Hydroxyformaldoxime [TT02].

Hydroxyformaldehyde [TT02].

Hydroxyl [CUS00].

Hydroxylase [HLC09].

Hydroxymatairesinol [SH09].

Hydroxyproline [BISB02, PRKP05].

Hyper [Mar03, vGGB00].

Hyperconjugation [CPDZH08].

Hyperconjugative [BPC01].

Hyperpolarizabilities [MO01, CJK02, LWZ09, Tor02].

Hyperpolarizability [Gan09].

Hyperpolarizability [Gan09].

Hypersurface [PSC01].

Hypersurfaces [PSC01].

Hypochlorous [JKM08].

Hysteretical [LD05a].

Hypoxanthine [KKMMS01].

Hypoxanthine-caffeine [KKMMS04].

Hypoxanthine-caffeine [KKMMS04].

I/O [SSL02].

ICFF [KTA03].

icosahedral [Ell07, LML00, OSA06].

IDE [Gan09].

IDEA [DBGV07].

ideal [Pan07, STSF02].

ideal-gas [STSF02].

identical [CSD05].

Identification [CP09, FWH07, KS05b, PPX01, SL0909].

identify [LHJ06, ZS04].

Identifying [CCJ09, DBI02, CLS09, HLT05].

identity [JSR07, Nee03, RC04].

idiosyncratic [CMCB08].

II [AC706, DPT03, DF04, FNP06, FKS09, GP05, LPP06, NK06, Sha02, TGGP06, WM01, BHW00, BA04b, Ber03, Car02, CSB08, EBD01, EKB02b, GGB07b, HZ06b, Ish03, JJB02, Kle03, LLA01a, LFZS04, LCDA03, LMF06, MB00, OBB05, PDB04, PV03, Rud05b, TUM03, TCR02, WHP02, WHN03, WFR08, vEMK01].

III [BB08, DF04, FR05, KPR04, VHR07a, YIN03, CCB04, CG05, KEB04, LAA01b, LCGA03, ZFL05, eV01].

Illustration [KS02a]. image [IC08, XWC09].

IMiCMO [MS01].

imidazole [JKM08, PG06].

imidazoline [XKG05].

imide [CIX09].

immune [WCS09].

immunoglobulin [Kr603].

IMOMO [VM00].

IMPACT [BC505].

Implementation [AKN07, CKW09, DRMD03, KBT03, LI07, PZH04, RGN03, SVO9, YTH07, BMRDB01, BLMS08, DFH05, DBS08, FRD08,GY06, JNV08,
Implementations [FL08]. implemented [HP01, MP03b]. implementing [OR05]. Implications [BBHD04, BLL+06, GL04a, JS07a, JZD+09, KTA03, Kr06, Lab08, MCM04, PZ04, PPS08, SBLK01, SL06, WL09a, ZGFL01]. Importance [CGBF05, ENM04, ZM06, HLC09, JW06, OCB02, PMPGP05, PMM05, TS05]. important [CSU05, EDAJ04, Tor02]. improper [TNS00]. improve [FSM09, XLT07]. Improved [CN03, CLA00, Gri03, HQ02, HK08a, HK08b, LC01a, LC01b, CMBC08, JS07a, JZD+09, KTA03, Kr03, Lab08, MCM04, PZS04, PR04, SD+01, STSF02, SHK+05, VZM+08, LC01a, RCJ02b]. Improvement [SM08b, UKN04, Nee03]. improves [CLWL09, RK05]. Improving [BUMCMRL00, Bie04b, GF08, LJ04, LW04, GRO+03, GP06, SMG09]. in-core [FR06]. inactivation [PFR04a]. incidence [YWH03]. InCl [ZL05]. Including [IC08, AK07, DP03, DP04, Gri04, Ish03, LB08, S09, Wil01a]. Inclusion [HK08a, HK08b, PWHF+03, PWHF+04]. incomplete [FHW+07, Ish04]. incompressible [ZHMW09]. incorporate [KTA03]. Incorporating [CM06]. Increasing [ZW09, BT00, LI07, YAC+02]. independent [FV08, OTL08, Van02a]. index [COS01, JLF03, MBH+02, PVdB00, Pog03, YWH03, YWH04, YWY07]. indexing [HWDB03]. indicators [BWW+08, HIM07]. indices [BL03, CGM+08, FZL07, FMP+08, FVB08, FS+04, GDPCPU07, MGMM07a, MGMM07b, May07, Rao00a, SPGS08, TSMG01, TSSG08, WMW03, WW03, WMW04]. indium [ZL05]. individual [ZM06]. INDO [PBZ02, TY03]. INDO/SCI [TY03]. indole [LL01]. induced [CGB03, CMBC08, EDW07, IM07, HHP04, KIFK07, LBG+09, LBG08, MLA00, PSF+08, RSN+02, ST01, ZALM03]. Induction [HK08c, HK08d, ZOJ+06]. Inductive [BE07]. inelastic [BACJCT01]. inexact [Har04]. inexpensive [KFZ03]. infinite [DA01]. Influence [GSB09, JS07a, JTO8, LZA02, BGC+09, SBH02, SLRC01, DB06, EL09]. Information [Ham07, GCB03, HTKG08, HP05, NL08]. information-bearing [NL08]. infrared [CVR08, KDC03, LDM+09, MGLD00, TDH06, Zer08]. Inherent [BYQS03]. inhibition [PFR04b, WC08]. Inhibitor [VVS07, BMFT08, CWV+05, FPG+06, MBC08, SVV+08]. inhibitors [AJNG01, AG00+02, APG05, AVS09, LLL+08, LZ05, PB06, RGP+07, VL09, VVS07, WYS04, WH08, ZW09]. inhibitory [DD08]. inhomogeneous [MAM07]. initial [MM03, MABM09, Qua07, UNM+01]. initialization [FKF+08]. initiated [RAGL09b]. initiation [GGGLL05]. initio [AJ03, AM02a, AM02b, AN06b, AS01, BG03, BG00, Bl08, BSB05, BS01, BL06, BLO+02, BSY01, BZL05, CJ00, CPM03, CUS00, CU01, CUSS03,
GGP09, Gon07, HLC09, HA04, HZ06a, HZ06b, IINK09, IB04, JWB05, KF02b, KH06, LHJ+06, LCC09, LZ03, LS08c, MM05, MMLC05, MCF07, NK06, Nil09, PG01, PC0+07b, PC0+07a, PK05, PNG08, RZWS07, SOOF05, San01, Sha05, SS0+09, SWV+05, SG01, SL06, SDL07, SMV+09, UTT+04, VW03, WR6+06, WPH+07, Won09, YT03, YTH+07, ZTS09]. interactive [DFGB09]. interactively [SB01]. Interatomic [RD06, AMR04, SS00, SPT07]. interconnected [SB08]. Interconversion [OO04]. interconversions [FD03]. Interesting [Kri09a]. interface [CW02, DPDG05, FO0+04, GKR08, HHBH00, HZX04, JKI08, KKG+09, LLL03, LPB03, PHJ+08, SWW04, TDMSD+08, ZCS04, DBGV07]. interfaced [FKL+06]. interfaces [BSH07, ZZTS09]. interfacial [CW02, MWL+08, PHJ+08]. Interfacing [WHG+07]. interior [SYC08]. interlayer [ALC08]. interlayers [DJT08]. intermediates [BLO+02, BMTFR08, IGL07]. Intermolecular [PSC+01, AS00, CM3+04, CLC09, FOA01a, FKH+06, FKH+07, MAF+07, GGP09, GS04, IGW07, KS05c, LZ03, Mas04, PMPGP05, RRCA08, SPDS01, SJW09, UTM+02, UTT+04, Wil01a, Wil01b, ZDS+05]. Internal [EA06, BHH+09, CFD03, COM+04, DHH+05, DHH+08, DHH+09, FOA01a, FOA01b, FOA01c, FOA01d, FOA01e, FOA01f, FOA01g, FOA01h, FOA01i, FOA01j, FOA01k, FOA01l, FOA01m, FOA01n, FOA01o, FOA01p, FOA01q, FOA01r, FOA01s, FOA01t, FOA01u, FOA01v, FOA01w, FOA01x, FOA01y, FOA01z]. Internal-rotation [DHH+05]. interparticle [PK05]. Interplay [EFQD09, SP05]. interpolated [YK08]. interpolation [BB05, IS03]. interpretation [CP00, HLS07, VM07]. intersection [SSHT03]. intersections [IK00]. interval [LS05a]. interwall [ZvRSC08]. Intra [FOA01a, FKH+06, FKH+07, MAF+07]. Intra- [FOA01a, FKH+06, FKH+07]. Intramolecular [GKT04, HA04, PG01, TFZRG01, AGK03, BA03, BA04a, FDSA00, HRKB03, HK08d, Li01, NHM05, RP02, SWW+05, VIP+06, ZDS+05, ZW09, ZHO8, Kle02]. Intraprotein [MLJ03]. intraresidue [IB04]. intrinsic [JS07b, JT08, YGZZ05]. intrinsically [NAT07]. Intruder [CW09, WCFH02]. intuitive [PP08b]. invariant [Est07, ZLY07]. Inverse [BR03, MLL08a, Nil09]. inversion [KSTC01, RC04, ZSE08]. investigate [DWN01]. investigated [HN02, Kle03, YH09]. Investigation [LZEC09, YTH01, AS06, BL00, CW02, CHA+07, CG08, FG03, GS04, Hir08, JH01, KYFW07, LH02, LS08, NS08, PV07, QZZ03, QZL+04, RM07, RC04, Ry09, SL04, TGGP+00, TFZRG01, UCT+03, WL09b, WLZ+07, ZXY08, ZKZ+07, ZHMW09, ZGX07, RGB03, JBGK08]. Investigations [JP09, WG02]. involvement [BLO+02]. involving [LL01, MM05, ZGX07]. iodides [CM09]. iodine [GWM+00]. iodobenzoylphosphonate [GWM+00]. Ion [DAM08, BM08, Dra00, EL07, FHR07, FL07, GWM08, Gor01, IvS06, KPR04, Kri08, Kri09b, MSBS01, PPS08, PHR08, RC04, VRH07a, VHR07b, ZW09, dOMS01]. ion-pair [RC04]. ionic [Ang09, BM08, BSG07, BJK01a, CFC+08, DMJ05, GGT08, HTN03, LR03b, Loe03]. ionizable [OS06]. ionization [GS09, KFD06, RTG00, SVT09]. ionospheric [LSHR04]. ions
[JVVK09]. Kr [CMJ08, CGB03]. Kroll [YH09]. Krylov [Har04]. krypton [CVVB04].

L
[Bac09, HT05, JPF+00, PC00, AGO+02, HT05, HJCP01, NYK+09, OYK+09].
L-2-haloacid [NYK+09]. L-captopril [AGO+02]. L-peptides [OYK+09].
L-phenylalaninamide [HJCP01]. L-valinamide [HJCP01]. La/SSB [KVS+06]. label [VCM01]. labeling [SN00]. lactamase
[AGO+02, APG05, SDM02]. lactamases [ESM06, MK02]. LADH [DMC05].
LaN [VP08]. Lanczos [MO01]. Landau [GHH07]. landscape
[IGNH03, PAT+09, SPL+02]. landscapes [OKH+02, SSB07]. Langmuir
[BRS00]. lanthanide [AB00, FRS05, RMP01, SNM+06, VMA03].
lanthanide [RD06]. Lanthanum [AB00]. Large
[WCF04, ARL01, AB08, AS00, BG03, BP01, BdPRMAI00, BME05, CJK+02, CDD+02, CG06, DMN03, DJB02, Ell07, FZL07, HB09, HSM06, IME02, IS07, JO02, JW00, KS05b, KK+09, KK01a, KH06, LMJ02, MKGA06, MH09, MHW04, MH08d, MPF00, ME06, NRKH02, PJF+03, RRS07, SYC08, SSL02, TY0+02, VSK+04, WWL+09, YCS07, vGGB00, WS07].
large-amplitude [KS05b]. Large-scale
[WCF04, DMN03, JO02, KK01a, MH09, MHW04, MPF00, ME06, RRS07, SSL02, TY0+02]. larger [VKP+08].
lariat [ZWY+09]. laser [Sha02, KZW+05]. latency [KVF+07]. latter
[LPK07]. Lattice
[OGH05, SG01, HP01, KWK+02, KWK+02, EF02b, LJKL08, MH08a, SCC04, SYC08, TK08, VGDS08, YCS07, vE01]. law
[Sch00]. LCAO [EBL+08, EL09]. LDA [RLD09]. lead [RS07a, RS07b].
leads [PPXP01]. learning [YCW+09]. least [CSD05, Go09, LLZL09].
least-square [LLZL09]. LEDO [GKH05]. legacy [Sha07]. Lei [Ano06c].
length [CRC+08, DR09, JPCA08]. length-frequency [DR09]. lengths
[PSC+01]. Lennard
[CYM02, FSFK05, Pul05, SCC04, SYC08, YCS07]. Lennard-Jones
[CYM02, FSFK05, Pul05, SCC04, SYC08, YCS07]. lesion
[Pin01, SHD+08]. lessioned [Pin01, Pin03]. Letter
[BFS07]. Letters
[BJW12, WM12, vLB012]. level [BUMCMRL00, BLT03, BL00, DPM09, JMD+02, mJlZsLyL07, KK08c, PFJ+03, RC04, TBG00, TST+08, UTM+02, WyLG+09, WS05b, WLL+03, ZZL04, ZWL+05]. levels
[BACJCT01, Cu04, DJB02, PFJ+03, WW03]. Lewis
[BHTCG07, Gr07, Sha07, Sim07]. LF [PWHF+03, PWHF+04]. Li
[CRC+08, GBDFP05, JW12, HDO+02, LWK08, LWW+06, LAT05, WWT08].
libraries [AL01, KV00, LZ05b, ZMZ09]. library
[CRH+07, FAB+00, KSM05, OTL08, SH07]. LiF [EL09, UM03]. lifetime
[CHA+07]. Ligand
[MKT04, AM06b, BSP06b, BGC+09, BS08, BMSC01, CGB+09, CLH+07, CN05, DFH05, FOO8, GZM09, HZ06a, HZ06b, HW09, JZD+09, KS08, LW+09, Mue01, NR04, NMAT01, OFIK09, PWHF+03, PWHF+04, RK05, Ru007, SOOF05, STSF02, TFA04, TJE03, VGGM05, XZZ04, YK00, Yan04, ZGL01, ZWS+02, BDW00, HLC09]. ligand-charge
[BSP06b]. ligand-protein [VGGM05]. ligands
light-emitting [LFR07]. lignin [PS09b]. LiH [McD03]. like [BCIB05, DHW00, DBI02, FZL06, JD09, Kut07, LAEL01, PRKP05, WL09b]. limit [MV06, MLL+08b, PSC+01, SAS05, Var09]. limitations [BYQS03, LFEdL06, PRDS08, MFB04]. limited [Ano05b, Sha05]. Limits [OV03]. line [RHL09]. Linear [Con02, DLWV07, KDG09, LMJ02, OS06, OFIK09, SKDO08, vdVGDJ00, AT02, ABÂ04, BH03, BPCD07, CC09, CGMPT+08, GCDL05, Gol09, GGLR00, Har04, KLM+09, MV09, McD08, Oos09, PK05, RI07, RS05, SS+03, TCR+02, vGB00]. Linear-scaling [OS06, SKDO08, GGLR00, TCR+02]. linearized [ABWT09]. link [GdAcV+07, KS02b]. linkages [SDL+09]. linked [CMD+04, CHRL09, FS98, FS00a]. LiPF [BSJ01]. lipid [HNL08, RGG08, SSM08, WC09]. Lipkowitz [Sta00]. lipophilicity [DMC05, DLHC06, DLHC06]. lipoxygenase [TGLL07]. lipoxygenase-1 [TGLL07]. LiPt [LWK08]. liquid [BM08, CC07, EGSG00, GDV03, GJK00, HPL03, MN02, MM07, NL07, PHJ+08, PB04, POJ01, YGLvG06]. liquid-state [POJ01]. liquids [CF04]. list [PABK03]. lists [KUB07]. lithium [HXD08, LWLS07, RC04, SLRC01, YSA+03]. liver [CMCB08]. LMO [BY06]. Local [Din00, LYS08, FS98, FS00a, JHPRSM+05, KMA+07, LMJ02, MA09, PMC08, RUPH06, SL09, SEKS09, SB08, TT05, TSSSG08, VKCK09]. localizability [BK08, BWW+08]. Localization [Che01, ALTB06, FS02, FSS00, GBJ03, PP08b, PA05, PAS07, PC05, SFC04, ST01, WMW03, WW03, WMW04, SHBD05]. Localized [ABF+03, AB09, Bac04, Bac05, Bac07, BME05, FMSA06, GFS05, ITN+05, TT01]. locally [TYO+02]. locate [ABBC01a, ABBC01b, Bo01, GMA04, MP03b, Qua01]. locating [WSM+09]. Log [Tot04]. London [Lab08]. Long [RP07c, CCSJ00, CPC+00, CEP07, CSRST04, Gri06, KSS08, LYS08, MN02, MBC08, RLP08, San01, VVBV02]. long-duration [CCSJ00]. long-range [CEP07, Gri06, KSS08, MN02, RLP08, San01]. long-time [CPC+00]. lookup [Nil09]. loop [CSJ04, KK01a, Mak08, OFB08, PRT+07, PRT+08, TLKT00]. loops [CSRST04]. LoProp [SKK+07]. Low [DPT03, MG06, AG00, BS05, GS03, KUB07, KK01a, KK01b, LAR+03, LB08, LS08, PFJ+03, PRSMV08, Rao00b, Sha02, WS02b, ZL05, ZL07, ZL09b, dSVA+09, BS08]. Low-DPT03. low-energy [Rao00b]. low-level [PFJ+03]. low-lying [LB08, ZL05, ZL07, ZL09b, dSVA+09]. low-mode [KK01a]. low-resolution [BS05, WS02b, BS08]. lowest [FDSA00, OSA06, XZ04, ZO04]. lowest-lying [FDSA00]. lp [LAR+03]. lp-RS-HDGR [LAR+03]. LR [ZWB09, NSO+07]. LR-MMPBSA [ZWB09]. LSCF [FAR02]. Lu [SNM+06]. lumiflavin [CNN07]. LUMMOX [MS04]. lutetium [AB00]. lyase [PMM05, ČJPZS08]. lying [FDSA00, LB08, PRSMV08, ZL05, ZL07, ZL09b, dSVA+09]. LYP [PDS01]. Lysine [DJT08]. lysozyme [HN02].
M [Bof01, GPSP06, JJK+00, LYZ+08, OS08, Qua01, WWC+05, JJK+00, LMGR06, OS08]. machine [CLS+09, HL08, LJZ+07, YCW+09]. machines [CLXC02, QLHL09, YMT04]. macro [Wou00]. macrocycle [RRZA08]. macrocycles [FLOD07]. Macro cyclic [SCG04, KB02]. macromolecular [ARA04, Con02, EA06, FM00, JO02, KS01a, KHY00, RP07d, ZBS03]. macromolecules [BVW04, HMWC03, YH06]. macropolyhedral [ZZZ+06]. Macrotricyclic [CW02]. Magic [KZW+05, HXD08, KKJH08]. magnetism [Hua09b]. magnetizabilities [YH07, YH09]. magnetizability [CDL06]. magnets [FKRE08, SM08a]. MAGPACK [BACJCT01]. main [Din00, JGH00, LW07]. main-chain [Din00]. macingroup [SRB06]. maingroup-element [SRB06]. Maintaining [LFBSK07]. maleimide [RP09]. malonyl [LLL+08]. malonyl-CoA [LLL+08]. maltose [SWBM08]. Manager [FCK+08]. manganese [AZM03, CWY09, GK09, LMIF06, LS05b, RJLR06]. Many [Loe03, BM08, TKH07, YCYX03, LR03b]. Many-body [Loe03, TKH07, LR03b]. many-electron [YCXY03]. map [MLL08a, SKGS00, HLTLP09]. mapping [FKZ09, RLA01]. maps [PRT+07, PRT+08, TTB01b, WD04]. Marchi [ANO06b]. Marcus [BLN01]. Markov [BHG03, CPUGD09, CMGDAC+07, DLW06, FWH+07, HLT+05, SK09]. Markovian [YCXY03]. mass [GM04, Gor01, KZW+05, LHJ+06, ZWZ09]. masses [CN03]. Massimo [ANO06b]. Massive [TP01a, RLA01]. massively [DGHR02]. master [FR06, FS00b]. master-slave [FR06]. matching [SMM+08, VSW+03]. Material [JW12, SLHW09]. materials [BCF+09, Haf08, LLXS02, LMRVFH+09, Tie09, XK08, YPNE09]. mathematical [DDVD09]. matrices [AT02, BDPRMAI00, CZA03, LSAS01]. matrix [CGSDST06, ELL07, GHHO07, IS07, JCA+02, LI01, NKIS02, NEE03, RS05, RRS07, RSS09, SK09, SSB+03, TYO+02, UHNO09, YWHZ03, vDSSvA04, vW06]. Matteo [ANO06b]. matter [ASDP+06]. maxima [MSS+06a]. Maximal [GCDL+05]. maximization [BWI+02]. maximizing [AM07]. Maximum [MVE02, SC070, HXD08]. MBO [CPC+00]. MC [HMD06, MLG04]. MCDP [SMG09]. MCDP [LAEL01]. McLafferty [NSB08]. MCM [NCO+05]. MCPRO [JTR05]. MCSCF [IR03]. MD [KIM+09, MDA08, ALB09, BMRF01, CADW03, HRR05, HXY05, PHRR08, WRBV03]. MD-based [BMRF01]. MD-GRAPE-2 [H605]. MDGRAPE [KAK+09, NYTH09]. MDGRAPE-3 [KAK+09, NYTH09]. MDSimAid [CHM05]. mean [GMA04, HFS03, LHI09, MMLC05, NMA01, RNG03, YCYX03]. meanfield [KRM+02]. meaningful [AE06, Bud07]. means
measure [XSHC06, ZHH09, PDC+08]. measurement [YZ04].
measurements [KBLP09]. measures [BDW00, DW08, Ham07, Leh06, PYEA03, PCA+08, PDC+08]. mechanical [AVB00, BSBO2, CLP09, CGBF05, CCK01, COL+06, DWCT03, ECA06, ESM06, EBD+01, FHRR07, 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, DFW05, DWC+03, EC06, FEVM01, GCD+08, GS04, GKT04, GP05, HWTL03, JCHS07, KLB03, KZRO03, LL00, LLA01a, LLA01b, LLA01c, LLA01d, LLA03, LSWB00, MLA00, MFB04, MPF00, OSIS03, PRKP05, PS09b, PWHF+03, PWHF+04, RMP01, RSE07, RP02, RO00, RM00, RGP+07, SS00, SHD+08, TGF+00, TFZRG01, TT05, VSW+03, XOW+00, YSA+03, ZSK07]. mechanisms [BDW00, RSE07]. mechanics/molecular [MPF00]. Mechanism [CJK+02, LWY+09, PFR04a, Ra00a, AM07, AGK03, BTP09, BLO+02, BS03, CGB+09, CBS+03, DBS07, HP04, HLB09, mJlZsLyL07, JDWS06, JH01, LMG+09, LLP06, LL01, LDT+02a, LDT+02b, LYZ+08, LFS+07, MCK05, Mui05, PGN03, PFR04b, PS03, PMM06, wQZsLyZ02, QZZZ03, Rjas06, SMK00, gThDjL+01, WDWS06, WCH09, WXX03, WJX+08, YQQH09, ZLSS04b, ZLSS04a, ZLSS05, ZLSS06b, ZKZ+07, ZGZX07, GVATG03]. mechanism-based [PFR04b]. mechanisms [AGI+00, AGI+07, BS06, CCCJ09, CG05, ILKR09, KZ09, KKJH08, LLK06, MK02, NS08, RC04, Sie01, TMBM02]. Mechanistic [BMTFR08, SGS03, TT02, Ana06a, ST06, WDS06, XDS06a, ZLSS06a]. media [HLLN06, MIM02, SMK00]. mediated [HIA03]. medium [FZL+06, HXX08, LF04, LFZ04, SHH07, ZFL+05]. medium-resolution [HXXL09]. medium-sized [SHH07]. melatonin [CK+08]. mellitus [PS09a]. Melting [LML+00, KT02]. membered [FJ08, ZW09]. membrane [ALB09, CJDK09, DAK08, FCP+04a, GAS04, ILKR09, JM07b, LPB03, MHJ06]. membranes [Ike04, SM08, WC09]. membranion [Ana00]. memories [WHRG08]. memory [TYO+02]. mercapto-carboxamides [TFZRG01]. mercapto-carboxylate [APG05]. mercapto-pyridine [YXZ+04]. mercury [FNP+06]. Merging [PJPJdPRMI07]. Merz [JVVK09]. Merz-Kollman-Singh [JVVK09]. mesh [BYQS03, KM00, KSY+00]. mesoscale [RPMP03, ZBS03]. Mesoscopic [YPNE09]. Met-enkephalin [ZCL09]. meta [DDBP09, ION07, ZTP+08, Gau09]. meta-di-Fluorobenzene [ZTP+08]. meta-generalized [IO07]. metabolites [PCMG09]. metabolizing [VB09]. metabolotropic [FTLV01]. metadynamics [BBB09]. Metal [SGD06, ABYM08, Ana06a, Boc05, BTP09, BS06, BRV+07, BM00, BWI+02].
metal-catalyzed [HSWW00]. metal-free [CM09]. metal-organic [TAS07].
metal-porphyrins [LS02]. metal-rich [LWK08]. metallic [ALK08, KWK+01, KWK+02, SK08, WLX+05, WL09b, dVB01]. metallo [AGO+02, APG05]. metallo- [AGO+02, APG05]. metalloenzyme [BDM04]. metalloenzymes [Sie01]. metallofullerenes [KSN01]. methanol [CCK01, YGLvG06, ZH08, ZWP08]. methionine [BTP09].

Method [KFB05, MO01, YGGZ05, AKN07, ABÅ04, AE06, Ami00, ATMK03, AB09, Ano05b, Ara04, BL09, BWP07, BP01, BVW04, BCN07, Ble04b, BH03, BF04, BM00, BGC+09, BHG03, BHH+09, CC09, CCL06, CSJ01, CG03, yCkHmY08, CRG01, CPC+00, CAG07, CA04, DPT03, DRMD03, DPRR05, DMLI05, DDM04, ECM03, FOK+04, FKL+06, FII+07, FÀ01a, FAR02, FS00b, FSR05, FRLN09, FKU+05, GMA04, GS09, GY06, GB04, HD04, Har04, HFS+07, HHS+05, HUFW07, HUFW12, HQ02, HDT+07, HSWW00, IK09, IR03, IK00, JO02, JVV09, KKY01, KDG+09, Kar01, KTA03, KN04, KM00, KLS02, KKC05, KSY+00, KK08c, Kolo4, KIM+09, KB099, KLM+09, KCO+1b, LSO04, LRW03, LR06, LWX07, LZZC09, LWX+09, LCSZ09, LZ05b, MLL06, MKGA06, MTK04, MBM+00, MCF05, MSH+06a, MHO8b, MG00, MS01, MY08b]. method [MPF00, MRS+07, NIK02, NA06, NGTB03, NG04, Nye07, OM04, PHJ+08, PAK03, PMC+08, PSZ04, Qua07, RNG03, Ra00b, RSE07, RLR+04, RL05, SK09, SMAdV00, Scho, SCC04, SYC08, Sha05, SF05, SG07b, SWZ04, SV09, THH01, TFN04, TVL+03, TY03, TKN+08, VK06, VZM+08, VM00, Vya01, WSO5a, WCC08, WW03, WLZ+07, WL00, WB030, WM04, WX09, XL02, Yan04, YZ06, YCS07, YAC+02, YH06, YH07, YH09, YXL+09, ZWS+02, ZL09a, vdVGD00, JBB00, KT029, SRC03]. method-based [KIM+09]. methodological [FDSA00, MFR07]. Methodology [KSL02, SPL+02]. Methods [SB01, AJ03, AGMPRG+08, BB05, BL05, CMGl+04, CG05, DLD+02, DB07, DNM03, DBM03, DDBP09, FOL+04, FO08, GHLK+02, GH07, GY08, GD09, GPN01, GGLR00, GHBB04, HTKG08, IB04, JFG04, KK08b, KBL08, Kle02, Kle03, KB09, LM07, LMB08, LLS03, LW06, LHP01, LK03, LKW04, LZF+09, MN02, MZ05, MBWP03, MHT01, MC06, OFB08, PDC+08, PSMB05, Qua04, RSSK03, RCJ02b, RK04, SAM06, Sch03, SBl05, SYC03, STH02, SE08, SDL07, SSB07, TBG00, TCR+02, TBGRJ04, VMA03, VC04, VMF+03, WMGK07, WMW03, WMW04, WSM+08, WCL05, WM01, YLL+09, ZM03, vDSSvA04, LSAS01].

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methoxycarbonyl [KK09]. Methyl [CADW03, CCK01, DBM03, DMN05, HT05, RC04, WLX+05, WDZS07, WSM+08, WLL+03, WC08, ZLLS05].
methylacetamide [MMPK01]. methylacetylene [ZKZ+07]. methylanine
[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 [WZZ+09, AS06, LST08, ˇSBL05]. Mg-porphin [ˇSBL05].
mGluR1 [FTLV01]. MgO [SBG09b]. MHz [CMD+04]. MICCs [YGZZ05].
micelles [KS02a]. Michael [Ano00]. microcanonical [Rap06].
Microiterations [VMF+03]. microscopic [KJP+07, TVL+03]. microsolvation
[UM03]. microwave [ZGXX06]. middle [RPNJ07]. migration [HLB09, ZGZX07]. MILCH [BL09]. mimic [WMS06]. minima
[CA04, DLD+02, KG02, XOW+00]. Minimal [BWZ08, BVW04, Maz01].
minimization [EGSG00, OM04, Sen06, WG02, vEMK01, ABF+03, NCO+05].
minimizations [dSR08]. minimized [GLD08]. Minimum [AM06b, AJ03, CZB07, CY09, CY13, SBLK01].
minor [BCP03]. misfolded [CP08, WS07]. mispairs [SG07a]. mixed
[FA01a, HELM09, MPF00, MC06]. mixed-valence [HELM09]. mixing
[AMR04]. mixture [WG02]. mixtures [FBDG06, NL07, YGLvG06]. MLR
[HSMT04, LLL+08]. MM [GC04, LLL03, MK02, PB06, WHF08]. MM-PB
[GC04, WHF08]. MM-PBSA [PB06]. MM2 [KKY01]. MM3
[AD00, LSWB00, YSA+03, FH01, St05, SBH02, TAS07]. MM3/MM4
[AD00]. MM4 [CLFA07, LLA01d, LLA03, ACLD03]. MMPBSA [ZW09].
MMVB [GRO+03]. Mn [AZM03, GD06, BL00, PYS05]. MNDO [DC02].
MND0C [IK00]. Mo [LZZC09, ML00, DRAS04, DRAS05, LDMR01]. MO/
statistical [ML00]. mobility [HIM07]. MoCalc [DPDG05]. Modal
[ES00]. mode [EBAN07, HNR08, KSU03, KJP+07, KK01a, SFRS01, TVL+03].
mode-specific [SFRS01]. Model [CPML08b, Duk01, EL07, Van08, AB08,
ABBC01a, ABBC01b, ATM+07, APG05, BG00, BBHD04, BLL+06, BT00,
BCIB05, BB08, BLN01, Bo01, BLMS08, CFF08, CF04, CFC+08, CP08,
CP09, CRSB03, CMR+04, CMGDAC+07, CA07b, COL01, COL+06,
DLWW07, DHW+00, DAK08, EA08, EDW07, EKO+01, FKL+06, FCK+08,
FEVM01, FC06, FBNO08, FZL+06, FNP+06, GZL02, GL04a, GK09, GJK00,
GKTS04, GGT08, GWS+02, HB09, HPL03, HS01, HK08c, HK08d, HHP04,
IL03, JBBJ00, JBB02, JPF+00, JBGK08, KSB+02, KFZ03, Lab08, LRI+02,
LAR+03, LFZS04, LJ04, LSRH04, LR06, LK03, LK04, LKA01, MWL+08,
MMPK01, MCF05, MBC08, Nak07, NL07, OKE+02, PCO+07b, PCO+07a,
PMB04, PFC03, Pom04, Qua01, RMP01, Sen06, TJE03, TCT03, TGGP+00,
Tot04, TT02, VW00, VW04, VGDSU08, VP09, WCK00, WKYU01]. model
[WS05b, WEE01, WOC+03, WJX+08, XL02, XZ05, XLT07, YL09, YPNE09,
YJF06, vDSSvA04, FCP+04b]. modeled [PB05, vDSSvA04]. Modeling
[ECM+03, FR05, MCR08, Mck07a, Mck07b, MTB09, PSC+09, SEK09,
Sie01, BA03, BA04a, BZP09, BM08, BSH07, CLP09, ČJPZS08, DJT08, DNN05, EDA04, ENM+04, GL04a, Gor01, HBM06, HMSM06, HMMS09, HRZKB03, HP04, Hin00, JM07b, JTR05, KCL06, KS01a, KJP+07, KVS+06, KPZK06, LEK07, LLL+08, LFR+04, MMLC05, MBM+00, MPF00, OFB08, SPGS08, SGS03, SY+03, SS05, SPF07, Sto05, TTBM09, VBGL+00, XLC08, YKK09, ZBS03, ZMH+09, BBC+05]. modelling [PSHP08]. Models [JB04, AS09, AHGK09, ACM+06, CCK01, CPUGD09, CRGN07, CA04, CA07a, CCT+03, DNM03, DLG00, DR07, DDVD09, EC06, FWH+07, FK07b, GS09, GDV03, GS02, GDPCPU07, GDPP08, GS08, HMDs05, Hs06, HD06, HP01, HLT+05, HG08, HJCP01, JPF+00, KS02a, Kr03, LJKL08, Leh06, LS08b, LDTS07, MTE04, MA05, MC06, OGH05, OYH05, PA05, RSS03, RS08, RR05, SBLK01, Sch00, SSS+09, SR02, SKK+07, SB01, SL06, VBS09, WB04a, WB04b, WB05, WZXY07, YÇBM00, YGLvG06, YJF06, YKK09, ZLJS03, ZCL09, ZGFL01, ZLD09, ZWP08, TDH06]. Modern [PB02, FLK+07, Pra01]. modes [Gra07, LS02, 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 [RHMK03]. Molecular [AS09, BBG+04, BG07, BDW00, CLC09, CLFA07, CCK01, DJT08, EMP07, FEVM01, FPN+05, GJK00, HLBO9, Ish03, JTR05, KSB09, KAS+07, KLB03, KIM+09, LLA01a, LLA01b, LLA01c, LLA01d, LLA03, LSFB00, MLA00, Maz01, MO9, MS00, MST+08, NB04, Pin01, RMP01, RRZA08, SHD+08, SDM02, VSW+03, WEE01, YSA+03, YGLvG06, YK09, ZCS+03, ZWS+09, AM09, AR01, AS06, AG00, ALBO9, AD00, AGMPRG+08, ATMK03, AM06b, AB09, AGO+02, APG05, AS00, BG03, BP00, BR07, BA08, BB05, BWE05, BRDC02, BWZ08, BVW04, BT00, BSOB05, BME05, BSJ01, BPCD07, CM08, CC07, CDS09, CLC06, COS01, CW02, CIB05, CDD+02, CF08, CCSJ00, CGBF05, CF06, CF04, CPC+00, CR02, CCP04, CE07, CMD+04, CSU05, CBH+03, DvG00, DB07, DPT03, DFWH05, DFG09, PDPD05]. molecular [DSS03, DMC05, DLHC06, DK01, DWC+03, ESM06, EKBO2a, EKB02b, FSO9, FHR07, FG02, FO+04, FKL+06, FII+07, FBDG06, FLOD07, FAB+00, FKL09, FEV+09, FKE08, FNP+06, FRLN09, FUK+05, FKM+06, GL04a, GLP08, GKR08, GCVB00, GLMV09, GFS05, GL08, GRC01, Gly06, GS02, GS03, Gou07, GSDT09, GCD+08, GS04, GKT04, GKP05, Ham07, HB09, HHWG08, HUT05, HGB04, HH04, HEL09, HM08, HLS07, HSW01, HN02, HP04, Hin00, HIA03, HTKG08, HDO8, HW03, HTN03, IKN08, ITS05, IC08, Ish04, IK09, IKYM09, JS07a, JMD+02, JP09, JGF05, JFG04, JHPRS+05, KM02, KFPS03, KKG+09, KM00, KCL06, KE04, KKC05, KSY+00, KAK+09, KCK+08, KBL08, Kn00, KZRO03, Kol04, KIFK07, Ky01, KH06, K01b, Kri09a, KPR04, Kri08, Kri09b, Kr03, KKS04]. molecular
myoglobin [AZS+04]. myosin [HSWN01].

N [GR07, JD09, KYFW07, KSN01, LS08a, LWW+06, Lu09, Mck07a, Mck07b, OS08, Sin07, TK08, WDXS06, WD08, WJX+08, XWXC08, YHD+06, ZY01, ZXY03, RMHK03, XZ04, ZO4, CPC+00, DRAS05, FJ08, FH01, HDO+02, KKH+07, KBL08, Lu09, LKA01, McD08, Mck07b, PFC03, RFSS06, SN00, SRE08, WLL01, Wil01b, 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 [LSJ05]. nanocomposite [DJT08]. nanomaterials [GJL+08]. nanomedicine [PSCD+09]. nanoneedles [PSCD+09]. nanoparticles [CGG06, KEM08, ZWC+09]. nanotube [KK08c, XWL+09]. nanotubes [BG07, ZZvRSC08]. nanowire [KK08c]. naphthalene [CDPL09, HRG07, WL09b]. naphthalene-like [WL09b]. naphthoic [CMLS05]. naphthylisoquinoline [BMRF01]. native [BS01, yCkHmY08, DBI02, MMMY07, WS07, ZCL09, ZS04]. native-like [DBI02]. Natural [FLGW00, Bac07, GS07, LZ05b, Pu09, RD06]. naturally [CJW+09]. 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-native [ZS04]. near-neighbor [PABK03]. near-solute [YL09]. Nearest [HDF+07, HTKG08]. Nearest-neighbor [HDF+07, HTKG08]. NCB [GF08]. needle [BS01]. Negative [BLO+02].Neglect [Lai07]. neglected [WC04]. neighbor [HDF+07, HTKG08, PABK03]. neighbors [RP07d]. nematogenic [CLP09]. neopentyl [YTY07]. Nernst [DAK08]. net [BED02]. Network [KYL03, AG03, CLC03, Go09, GDPP08, GAS04, HMSM06, KEB04, LSY02, MVLG06, NINAT+07, SJJ+04, SPT+03, UHNN09, WX09, LMH+09]. network-based [GDPP08, GAS04]. networks [BMRB01, BSH07, FCK+08, KVF+07, LJJ+07, PS09a, RLA01, TCSM03, VGDSU08, dVB01]. networks-based [PS09a]. Neural [GA04, AG03, CLC03, Go09, HMSM06, KEB04, LJJ+07, NINAT+07, PS09a, RLA01, SJJ+04, TCSM03, WX09, dVB01]. neuronal [SBG+09a]. Neutral [DWS+09, ASS+02, Bac09, CYM02, DLR+08, EBDPM00, FCP+05, MT03, OSA06, PGG06, ROG00, VM02, Wan09]. neutrals [LLXS02]. neuron [BACJCT01, RMHK03]. nevirapine [AJNG01]. new-generation [YJJ06]. Newly [CRS05]. News [An04b, BACJCT01, DvL01, Gly06, JVVK09]. Newton [Har04, Qua07]. NF [FJ08]. NH [DMM05, LF02, DOMSL01, DRAS04, ITS05, JPF+00, KT08, KSTC01, LDMR01, MR02, Mck07b, PC00, SEK09, dOMSL01]. NHC [ZWL+08]. NHHN [LWY+09]. Ni [Bac09, KGL07, PNM06]. NiAt [ZL07]. niches [TP01a]. nickel [Bac09, GK09, LMF06, YQQH09]. nicotine [VB09]. nicotinic [GCD+08, SBG+09a]. NiH [ZL07]. NO [SBG09a]. niobium
[Tie09]. NiSOD [PMM06]. nitrate [CGB+09]. nitrenium [FG03]. nitric [JDWS06, LPP06]. nitride [UNM+01]. nitrides [LX07]. nitrido [Bac05].
nitrogen [GWM08]. nitrogen [BGC+09, WC08, XWL+09, ZLLS04a, ZLLS05, ZWY+09, ZMH+09]. nitrogen-containing [LLM09].
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, AGI+07, AGI+07, BPC01, BRDC02, CADW03, CMD+04, CMA+08, FO04, HP05, Kle03, KBLP09, MC06, P06, PC00, PF06, P06, Ri07, Rs09, Zpl07].
NO [LDT+02b, MG03, MG03, P06, P06, P06, P06, RAGLL09a, XDS06a, ZLLS06a].
Nobelium [HdMdS05]. noble [SRB06]. nodal [HYT05]. nodes [Kau07]. NOE [AGI+07, AGI+07, AGI+07, PF06].
non [GZ07, Gon07, SVT09]. non-bonded [GZ07].
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].
non-equilibrium [FZL+06, GG09, KK08c, LF04, LFZS04, OD09, YZ04, ZFL+05]. nonhybrid [DF04]. nonisomorphic [CRGN07]. Nonlinear [RLA01, BF04, BF07, Har04, HLFH05, MMP+07, WCL05].
nonlinearity [LPK07]. nonmetallic [ALC08]. nonnative [yCkHmY08]. nonnucleoside [AJNG01]. nonorthogonal [SMZ05]. nonparametric [HDF+07].
nonplanar [Din00]. nonplanarity [RKH03]. nonpolar [GZL02].
nonrelativistic [WL02]. Nonspecific [LPB03, RGG08]. Nonuniform [SHSF05, Bie04a]. norbornadiene [WXK08]. norm [RRS09]. normal [EBAN07, KSU03, OR05].
nose [BBG+04, QNF09]. Note [Ano04a, Ano04a, FBS09]. Notes [CDGS09, CDS09]. Novel [ILKR09, JLHF03, NL08, TRS02, WL09b, YWHZ03, CRK08, CMBC08, GZL02, GDV03, LXW+09, RO8, TY0+02, YJF06, ZNLL07, ZL09a]. novo [LEK07, VGO+07]. Np [Han01, Ike04, GHLK+02]. NPAT [Ike04]. NPT [Ike04].
NQR [MH08a]. NR [CPJ00]. ns [CMD+04, SO07]. NSAIDs [CMBC08]. Nt [ZNFL07]. nuclear [C09a, C09a, C09a, C09a, C09a, C09a, C09a, C09a, C09a].
Nucleation [BACJCT01]. nucleation [CKW09]. nuclei [CDPL09]. nucleic [CCK01, DP03, DP04, FZL07, FM00, HWTL03, JCL05, MB00, Nak07, OMNH08, PPYS08, RKH03, SYC03, SL04, SWR06, SHK+05].
nucleobases [FKS+09, SB08]. nucleophilic [BSB05, SB07]. nucleoside [Wil01b].
nucleosides [SA07]. nucleosome [VTT+08]. nucleotide [Mak08, MSF+08].
nucleotides [XWX08]. nucleus [FVB08, HDMDS05, HD06, HD06, IKN08].
NUCS [SHSF05]. nudged [AJ03]. number [CD509, HXDO8, KZRO3, KZWO+05, KH06, TGGP+00, WWL+09]. numbered [GYCZ04]. numbers [CDS09, HXD08, KZRO3, KZWO+05, KH06, TGGP+00, WWL+09]. Numerov [Bie04a, Bie04b]. Numerov-type [Bie04a].

O [BL00, GCCVB00, GSPS06, HYR06, ITS06, mJiZyL+08, KGL07, LZZC09, LM009, Mas01a, Mas01b, NA06, Owe05, PGNG03, PGRNG03, UCT+03, XWXC08, YHD+06, ZJM+07, ZY01, ZZZL04, ZZL+08, ZY03, Bao09, CCCJ09, DRAS05, Dib05, HM08, HDO+02, IS03, LC07, LW04a, LS05b, MGLL03, NyHN06, NHN06, RAGLL09a, RFSS06, SSL02, SRE08, Wli01b, YTY07, ZJX09, KZY09]. O-methylation [HM08]. O3LYP [BP03]. OB [NA06]. object [CRH+07, FL08, MVL+05]. object-oriented [CRH+07, MVL+05]. objective [WG02]. objectives [STCJ08]. objects [RSN+02]. observables [MG06]. observations [FWH+07]. observed [VBS09]. obtain [BVW04]. obtained [HFS03, VC04, WMW03, WMW04, WHH+06]. obtaining [Bac04, YGZ05, SK09]. occupied [HHW08]. occurring [CJW+09]. OCF [UTM+02, UTT+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, Gol09, Tot04]. octanol/ water [CSB+03, Tot04]. octet [GR07]. Odd [CC07, GYR04]. odd-numbered [GYCZ04]. off [HP01, LJKL08, XLT07]. off-lattice [HP01, LJKL08]. off-plane [XLT07]. OH [Dib05, Gog08, HTN03, IvS06, LW04a, Mas01b, WLL07a, CU01, CUSS03, GAI05B01, GCCVB00, GGGGL05, HTN03, KZY09, Kle03, KBLP09, LC07, LW04+09, Mas01a, MGLL03, Mu05, RAGLL09a, RAGLL09b, SEKS09, UCT+03, WLLS04, WLL+07b, WyLG+09, YLW+08, YLWL09, ZZL+08]. OH-initiated [RAGLL09a]. OH-rotamer [KBLP09]. OH-stretch [Kle03]. OH/Cl [YLW+08]. OHO [Wil01a]. OHS [JP09]. olefin [PPH07, YXC+07]. olefins [AVB00]. oligomeric [EL07]. oligomers [BSG07, CSJ01, Der09, LF07, SBB02, WCL05, ZOJ+06]. oligopeptides [MGJAARC00]. Oligovalent [KS02b]. OLYP [BP03]. on-the-fly [KMA+07]. On-the-path [CY09, CY13]. One [CR09a, BG03, Bac07, Bie04a, GKR08, KFD06, Kri09a, Lai07, LB05, ZWS+02]. one- [Lai07]. one-dimensional [Bie04a]. One-electron [CR09a, BG03, Bac07, GKR08, KFD06, Kri09a, LB05]. ONIOM [BGC+09, MDA08, MC06, VFF+03, XXKL03]. ONIOM-molecular [MDA08]. ONO [FJ08]. onto [NK06]. OOPSE [MVL+05]. open [CSV+07, FS02, PRSMM03, LLA01a]. Open-chain [LLA01a]. open-shell [FS02]. open-source [CSV+07]. opening [SRE08]. OPEP [ACD+03]. operating [DFWH05]. operation [PCA+08, SYC08]. operators [KRM+02, Qua04]. OPFMM [CRG01]. OPLS
...
[BTP09, DRAS05, GCCVB00, GGLL05, LB05, RAGLL09b, SS05, XPW09].

**Oxidative** [DGD+05, LL00, PMM06]. **oxide** [BSJ01, CFS+08, CCCJ09, JDWS06, JT08, LPP06, PV07, RRS06, SBB02, ZCS04]. **oxide/electrolyte** [ZCS04]. **oxides** [ZSC05, ZLLS05]. **oxidized** [CNN07, CR02].

**oxidoreductases** [CGS+03]. **oxidosqualene** [SGS03]. **oxo** [CN05, WJX+08].

**oxo-carbenium** [LSWB00]. **oxoguanine** [FPN+05, JM07a, Pin03].

**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, RPN07, RFSS06, Tot04, KZY09]. **P450** [AST06, HBM06, LCC09, ZAT07]. **P450-catalyzed** [AST06]. **P450nor** [LPP06].

**P450**s [OYH05].

**P** [Anhar] [GBDP05]. **package** [AGSF+05, BACJCT01, CSV+07, GSDT09, IM06, KSY+00, Ki01, KWK+00, MABM09, OTL08, PVdJB00, RMH03]. **package-independent** [OLT08]. **packed** [AT02].

**Packmol** [MABM09]. **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, CJD09, FZL07, KKMM04, 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, KC01a, ZW09]. **para-didehydropyridine** [KC01a].

**para-didehydropyridinium** [KC01a]. **para-hydrogen** [ZX09]. **paradox** [CDG09].

**Parallel** [BWP07, DOSG06, MBWP03, TGGP+00, UIHN09, ASWG07, Ano05b, AGSF+05, BP02, BWM+09, CR01, GBDP05, GS04, GKT04, GPK05, HHJ03, HHS01, IS07, IPN06, IPN07, KKC05, KOFF09, KVF+07, MVL+05, MGJACK00, NK02, NG04, Sha05, SPT07, TYO+02, TFZRG01].

**Parallelization** [GJK+06, PVdJB00, PV03, SZV+05, UKNS01, CCWH02, FOK+04, FCK+08, UKN04, VSK+04, vGGB00]. **parallelized** [TP01a, VK06].

**parallelizing** [SO07]. **parameters** [BLSM08, CRG01, CHMI05, HXLS09, MO09, OVMV04, SHK+05, FM00].

**Parameterization** [KB02, PNG08, SMM+08, TCT03, BGJ01b, FH01, JKL08, JGH00, LSWB00, MTE04, PB04, RKH03, TGLL07, VSW+03, WK01, JJ02, JYV09].

**parameterized** [GB04].

**parameters** [AAP00, AM04, Ano06c, ATBLS04, BBS04, BZL05, CYM02, DB06, DDVD09, FAR02, FSF05, FRS05, HPL03, KFNH08, KOML08].
KVL +04, KC01b, MMMY07, MSR04, MRC03, MLL +08b, MC06, OYH05, OMHR08, OBT09, PRKP05, RRCA08, SO09, SEKS09, SRCD03, SHD +08, SCF +09, TT05, TTB01a, VCM01, VIP +06, WZW +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 [AGI +07, CDS09, ESP04, GDPP08, LLA01d, vDSSvA04, AGI +00, Rud05c, vEMK01, vE01]. Partial [ike04, BS +01, 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, Gol09, RM07, TS05].

Partitioning [ACD +03, DVP +02, DVRP +03, HSM06, RP07a, VC04, WHN03]. path [ABB01a, ABB01b, Blo04, Bo01, CY09, GF08, GWM08, JP09, Kli01, Qua01, UCT +03, VGB08, WLPF05, WHG +07, CY13]. paths [FG03].

Pathway [LGB +09, WLL01]. pathways [AJ03, JW06, LZKT04, MA +07, Qua04, RAGL09a, RAGL09b]. Pattern [DGHR02, EKB02a, EKB02b, KE04, AGMPGRG +08, HWDB03, dGW01, EKB02a]. patterns [CGG06, Gor01].

Pauli [Ish03]. PB [GC04, WHF08].

PBCAID [QSS01]. PBSA [PB06]. PbTiO [ZYF09]. PC [Ano01b, BMRDB01, HSMT04, OSH03]. PC-GA-ANN [HSMT04]. PCM [FKL +06, CRB03]. PCs [HS07b]. Pd [GG +05, GBBH09]. PDDG [RCJ02b, TBGR04]. PDDG/MNDO [RCJ02b, TBGR04]. PDDG/PM3 [RCJ02b, TBGR04]. PDE7 [DD08]. pea [PS03].

PF06, WD04, MM05, OOO8, SSS +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]. CCI [ZLS06a]. CF [YLWL09]. C1 [YLW +08].

closure [SWR06]. continuum [LRI +02]. Cs [GLR02]. decomposition [ML00]. DFT [BRLS12, BRLS08]. dissimilarity [hYD08]. DQ7 [KVS +06]. electrolyte [ZCS04]. empirical [CYM02]. FE [AGK03].

four-centers [GYMN07]. fractal [Fan07]. free [BG00]. Ge [LLXS02]. GeH [LLXS02]. heavy [SL09]. HLA-DQ8 [KVS +06]. implicit [LS04]. Kohn [RRS07]. L [KOML08]. metal [MSBS01]. MM [CGBF05, MF00, AST06, CR09b, C05, FAR02, FMSA06, FSFK05, GWM08, GWM +00, HHBH00, HM06, HNR08, HRR05, HTN03, IV04, IvSV06, ITS05, ITS06, KHF +09, KPR04, Kri08, Kri09b, MBM +00, MSH +06a, MG00, ML03, NGTB03, RG02, SBG +09a, SN06, SMM +08, SVV +08, THHN01, TdMSD +08, VSF +03, WCC08, WHG +07, WC08, YZ06, ZWZ09].

MM4 [AD00]. Mn [BL00]. MNDO [RCJ02b, TBGR04]. molecular [CGBF05, FÁ01a, MF00, TCR +02, VHR07a, VHR07b, XLZ08, ZAT07]. MP2 [WD04, GKT04]. MRCl [KT02]. nonstable [GDPCPU07]. NP [GZL02]. one-step [Oos09]. order [MO09]. particle [BYQ03]. PM3 [RCJ02b, TBGR04]. polarization [YL09]. poly [BSJ01]. 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]. Peptide
[Adc04, DHW+07, HJCP01, JPF+00, OHNH00, 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, WCF04, Wil01b, YZ06, YÇBM00, ZALMG03,
ZC03, WHP02, KVS+06]. peptide/HLA [KVS+06]. peptide/HLA-DQ8
[KVS+06]. Peptides [CPML08b, Van08, Ano06c, BBHD04, BCP04,
BAH+02, CP08, DJ04, EA08, HHP04, IKYM09, LKJ+04, LLW02, LXL07,
MM00, MC06, OML+00, OYK08, OM04, PCO+07b, PRKP05,
PFC03, SJW09, WZW+06, YAÇ+02, ZW09, ZLD09, ZOJ+06, PCO+07a].
peptidomimetics [BAH+02]. percolation [Mei02].
Perfect [Wan09, OCB02]. perfluoro [FO04]. perfluorosulfonate [YSJ09]. perform
[ME06, WCK00, WHG+07]. Performance
[BM00, Cul04, CA04, DMN03, FOL+04, JM07b, KPKZ06, LLS03, RLDI09,
VB09, ZM03, AM06a, BL05, BRV+07, BLMS08, CCWH02, DF04, DB06,
DGI+08, FMP08, KWK+00, KEM08, KS05c, LWH06, MA09, NYTH09, SF07,
SCF+09, Sto05, SBH02, UKN04, WMGK07, 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 [CRGN07].
permittivity [GP01, PZS04]. permutation [SN00]. perovskite [WD08].
perovskite-type [WD08]. peroxa [BLO+02]. peroxidase [HBM06].
peroxidative [MR09]. peroxides [LLZL09]. peroxy [Dib05].
peroxynitrite [JM07a]. personal [May07]. perspective
[KRLD09, LMGO+09, PBF09]. perspectives [Fie02]. perturbation
[CWY09, CPML08a, CG05, DRMD03, JSR+07, FII+07, Gri03, IN08, LK04,
MRS+07, NUH02, Oos09, PMGL03, Pog06, QT+d+08, RSE07, SWZS04,
UTH+03, UKNS01, UKN04, Var09, WCFH02, WHH03, 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, FBDG06, FM00, GLMV09, JJK+00, JHZ09,
KS+02, KT08, KFNH08, KKH+07, LRI+02, Lee09, LB05, LLL03, MBF04,
Mas01a, Mas01b, MM02, Mor02, POJ01, PV07, wQZsLyZ02, QNF09, RRS06,
ROG00, SMGE08, SDvG01, SMKM00, TK08, TDH06, UCT+03, UNM+01,
WD04, XKKL03, XKG+05, YQQH09, ZALMG03, ZSK07]. phase-space
[QNF09]. phases [ALC08, CLP09, LXF08, SK05, XB08]. PhAST
[HHG+09]. Phe [VKP+08]. Phe-Gly-Phe [VKP+08]. Phen [ZWS+02].
point-charge [DWC\textsuperscript{+}03, GGLR00, SRB02]. points [BMLV04, BAA\textsuperscript{07}, DLD\textsuperscript{+}02, GMA04, HQ02, MP03b]. Poisson [WB04a, WB05, ABWT09, BHW00, BH03, BF04, BF07, DLG00, DAK08, FOL\textsuperscript{+}04, GPN01, GCD\textsuperscript{+}08, GGT08, H\text{ö}f05, HBW00, HBW01, KWWH07, LDG02, NYTH09, PZS04, SAT004, Vas02, VZM\textsuperscript{+}08, WB04b, ZGFL01].

Polanyi [Nye07]. polar [BAÅ\textsuperscript{07}, CYM02, CPML08a, EB04, F\text{"{A}}A01a, HLLN06, HSF08, JPF\textsuperscript{00}, PFC03, ZXYF09]. polar-neutral [CYM02]. polarizabilities [ZPL07]. polarizability [BP01, HK08a, HK08b, Mar03, Mor02, QCK01, QCK02, vGGB00].

Polarizable [CFK08, LLM09, Nak07, Ano06c, AGO\textsuperscript{+}02, APG05, BCIB05, COL\textsuperscript{+}06, DGI\textsuperscript{+}08, FKLU06, GWM\textsuperscript{+}00, GS04, GKTS04, GPK05, HHP04, JZD\textsuperscript{+}09, KSB\textsuperscript{+}02, Koi04, LJ04, MMPK01, MBC08, OR05, PWHF\textsuperscript{+}03, PWHF\textsuperscript{+}04, Pom04, RGP\textsuperscript{+}07, TFZRG01, WZW\textsuperscript{+}06, YGLvG06, FCP\textsuperscript{+}04b].

polarization [CGB03, CBH\textsuperscript{+}03, EDW07, GGLR00, HK08a, HK08b, KFZ03, MR04, Maz08, RP02, SL09, WL09a]. Polarized [EdlVR\textsuperscript{+}03, BSOB05, OBBS05]. poly [ASDP\textsuperscript{+}06, CHA\textsuperscript{+}07, CFD04, MGMM07b, Qua07, SBB02, ZALMG03].

poly-phenylene [ASDP\textsuperscript{+}06]. polyacenes [BPCD07]. polyacrylates [LZA02].

polyacetylene [PM02].

polyacids [KBLP09]. polyatomic [GGB07a, GGB07b, RLER04a]. polyanions [TP01b]. polyazidocubanes [JWB05]. polycoordinated [TGGP\textsuperscript{+}00]. polycyclic [Bor03, CA07b, FVB08, MGMM07a, VS08].

polyenes [MW09]. Polyethylene [BCF\textsuperscript{+}09]. polyketides [KB02].

Polymer [Mei02, BBG\textsuperscript{+}04, CZA03, DJT08, MM07, RRZA08, YS09].

polymeric [Fau01, JCA\textsuperscript{+}02]. polymerization [BG07, YXC\textsuperscript{+}07]. polymers [CFD04, CA04, CA07a, DC02, Der09, Din00, DDBP09, HM01, LAEL01, OKK\textsuperscript{+}02, SHH07, VIP\textsuperscript{+}06, YYW07]. polymorphism [VVBV02].

polyenal [HDBD04]. polymeric [HYR06, RRFC\textsuperscript{+}03]. polyoxoanions [LFR\textsuperscript{+}04]. polypeptide [Cri04]. polypeptides [CPML08a, IB04, KF02a, KF03, Nak02, VP09].

polyphosphate [MRC03]. polythiophene [CA07b]. POPC [JM07b]. Pople [Ano04a, EA08].

population [BLT03, BPCD07, Pul05]. population-based [Pul05]. populations [KBN02]. porphin [SBL05, SBL05]. porphycene [NyHN06].

porphyrazines [LS02]. porphyrin [AZM03, CHRL09, LPP06, NyHN06, NHN06]. porphyrin-fullerene [CHRL09]. porphyrins [CN05, LS02, LWH06]. portable [SH07]. positron [RGG08]. Possibilities [PRDS08]. possibility [LMGR05, LBG08, TT05]. Possible [HIA03, OCP02, WLL01]. post [WW03]. post-HF [WW03]. posteriors [SPDS01]. potassium [MCR08, MHS05]. potential [AMR04, AE06, ABBC01a, ABBC01b, BCNs07, BL05, Bo01, BBI\textsuperscript{+}09].
DMLI05, DMC05, DLHC06, DK01, FSFK05, FKRE08, HPP00, HRBKB03, HPL03, HFS03, IS03, IT03, JZD+09, LFK05, LMK01, LS08c, MMLC05, MCF05, Nak07, NG04, NMA01, PSC+01, Qua01, RD06, RNG03, RHL09, RTG00, SPD01, SS00, Sch03, SMGE08, SSS+09, SHH07, SG07b, SBB02, SJ09, TBS09, TLKT00, WCC08, WL09a, WCK00, WS07, YH06, YHD+06, ZCS04, ZZY07, ZZY08, ZGXX06. potential-derived [TBS09].

potentials [ATM+07, CLC09, CPUGD09, CKW09, DBI02, FAB+00, FNP+06, GK09, GBJ03, HZ04, HHHS01, HZ06a, IKY09, KHL+04, KCK+08, LK03, LK04, LLW+09, MCF05, MWE02, OR05, PML03, RLER04b, SMAdV00, 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, SWZ04, WW03].

precalculated [ZMZ09].

preceding [CSD05].

Predict [AVS09, CLC03, CKR08, CJDK09, DA01, ELK+09, FCW06, Go09, JIK09, KHL+04, KCK+08, KEH+02, KF03, KKS04, LCC09, NINAT+07, OFB08, Sch00, YCW+09, YYW07, ABÅ04, BFD02, CLF+09, CLA+00, DB06, EK06, GP06, GAS04, HEP+02, HSM06, HG08, KZY09, KL05, KF05, KF08, KEB04, KKE08, KLS08, KOFF09, KF02a, LEK07, LWX+09, LHP01, LLZ09, LWH+09, MFS+08, MB04, NCO+05, NLL+09, PJB+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, vEMK01, vE01].

predictor [Kol04].

preface [FA01b].

preferences [GSB09, KK09, LKJ+04].

preferred [DV02].

preliminary [KMH02, PMC+08].

Preprocessing [SHM04].

prerequisite [WHF08].

presence [LZA02, RAGL09a].

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, HZX04, Hua09b, KK08c, MLJ03, TK08, VP08, WLX+05, WZZ+09, WD08, ZXY09, ZHM09].

prion [IK09].

priorti [SPDS01].

prismatic [WL09b].

probabilistic [PJB+07].

probabilities [DP04].

probability [CFS03, DLW06, GCDL+05, Kn00, SK09, SCS07].

probe [CVR08, DMLI05, TH02, VSW+03].

Probing [PAT+09, WMGK07].

problem [ABBC01a, ABBC01b, Ano06a, Bofo01, CCL06, HLTLP09, Qua01, ST06, TKB07, XOW+00].

problem-size [HLTLP09].

Problems [You11, ABWT09, Mat03, Vis02, Woo01].

Procacci [Ano06b].

procedure [AM09, BR03, CA07a, DLS00, GP06, KBT03, RS08, SSL02, SMM+08, YÇB00, Zho06].

procedures [GT03, HSM04].
processes
processing
processor
processors
producing
producing
producing
producing
producing
producing
producing
producing
producing
producing
producing
producing
producing
prokaryotes
prolapse
proline
promising
promolecular
promoted
promotion
propagator
propanal
propanone
proargyl
propellanes
propenal
propene
properties
properties
properties
properties
properties-based
propylene
propynyl
protease
protease-inhibitor
protein
protease-inhibitor
protein

LFBSK07, LHJ^+06, LJKL08, LV08, LZKT04, LXW^+09, LL07, LW06, MFB04, MKT04, MG04, MH09, Mei02, MWE02, MLL08a, MHT01, MPF00, NMAT01, OBF08, OFIK09, PB06, PHR^+05, PC00, PFC03. protein [PSHP08, PMM05, PB02, PF06, PNG08, QLHL09, RI08, RSER09, RL08, RSK08, Ru0v07, SM04, SLC^+09, SWM04, SWV^+05, SN06, SR09, SM09, STCJ08, SL06, TLKT00, TGD05, VW00, VW04, VGO^+07, VGDSU08, VGGMM05, VZM^+08, WS05a, WS07, XZZ04, XSHC06, XLC08, XWC09, Yan04, YL06, YFS07, YPNE09, Yos02, ZP03, ZGLF01, 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, DWNB01, DMN03, DR07, DV02, DJ04, DJB02, DWC^+03, ES00, ENM^+04, FNP^+06, GAS04, HB09, HHHS01, HM02, HS01, HHW^+03, HL08, HJCP01, Ike04, IDMC09, IN01, KSB^+02, KT02, KKS04, LR03a, LJJ^+06, LKA01, MK02, MSF^+06a, MZL08, NAT07, OS06, OSHS03, OM04, PB04, PMB04, PRJ02, RON02, SL09, SPL^+02, SHBD05, SHS05, SMV^+09, VBS09, VZW^+06, WM06, WS05b, WHH^+06, XZ05]. Protocoll [AGI^+00]. Protein [SRB06, AGK03, BA03, BA04a, CXZ^+09, FDSA00, FO08, GWM08, HFHL06, LL08, LMGO^+09, LB05, MA05, PGG06, PCS04, SM06, WFHP01, WHP02, XKG^+05]. Proton [SRB06, AGK03, BA03, BA04a, CXZ^+09, FDSA00, FO08, GWM08, HFHL06, LL08, LMGO^+09, LB05, MA05, PGG06, PCS04, SM06, WFHP01, WHP02, XKG^+05]. Protonated [CPDZH08, ZDS^+05]. protonation [Bac05, CG05, DHM^+03, HP05, KFW07, WHF08, XZ05]. protoporphyrinogen [WZY04]. prototype [Ang09, CS01, ASDP^+06]. prototypes [SS^+09]. proximity [Agr03]. pruning [TSCM03]. pseudo [LL07, VDM06, XSHC06, XLC08]. pseudo-Jahn [VDM06]. pseudofolding [VGDSU08]. pseudoknots [DP03, DP04]. Pseudomonas [NYK^+09]. Pseudopericyclic [LFS^+07]. pseudopotential [FMAMVK06, LK03, VW03, vW06]. pseudopotentials [PSS^+04, PSMB05, SMD02]. PS13 [CSV^+07]. psoralen [NBNT04a, NBT04b]. Pt [DMN05, 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 [MDI04]. pVDDZ [Wib04]. pVTZ//MP2/6 [WD04]. PW [EBL^+08]. PyFrag [VGB08]. pyrazine [LWX07]. pyrazole [DMC05]. pyrazoline [LLK06]. pyrazolyl [HT05]. pyrene [HA03]. pyridine [CHA^+07, HT05]. pyridines [WRP^+06]. pyridoxal [LDY^+08, PMM05]. pyrimidine [LWX07, WXCC08]. pyrimidiny1 [WJX^+08]. pyrolysis [KKH^+07, XKKL03]. pyrope [ZWTP^+08]. Pyruvate [ČJPZ08]. pyVib [Zer08].

Q [BS08, KKW^+00, WHG^+07]. Q-Chem [WHG^+07, KWW^+00]. Q-Dock [BS08]. QCISD [ZK^+07]. QCT [DPM09]. QM
[CBF05, MPF00, AGK03, AST06, AB09, CR09b, CG05, FAR02, FMSA06, FSF05, GWM08, GWM+00, HBBH00, HBM06, HR08, HRR05, HT03, HTN03, IV04, IVSV06, ITS05, ITS06, KHF+09, KBLP09, KPR04, Kri08, Kri09b, LLL03, MBM+00, MG00, MLJ03, NGTB03, RG02, SURG06, SGB+09a, SN06, SMM+08, SVV+08, THHN01, TdMSD+08, VMF+03, WCC08, WHG+07, WC08, ZWZ09]. QM/FE [AGK03]. QM/MM [CBF05, MPF00, AGK03, AST06, CR09b, CG05, FAR02, FMSA06, FSF05, GWM08, GWM+00, HBBH00, HBM06, HR08, HRR05, HT03, HTN03, IV04, IVSV06, ITS05, ITS06, KHF+09, KPR04, Kri08, Kri09b, LLL03, MBM+00, MG00, MLJ03, NGTB03, RG02, SURG06, SGB+09a, SN06, SMM+08, SVV+08, THHN01, TdMSD+08, VMF+03, WCC08, WHG+07, WC08, ZWZ09]. QM/QMPF [PHRR08]. QMD [KMH02]. QM/QMPF3 [DGI+08]. QM/QMSAR [DMLI05]. QSAR [DHW+08, DHW+09, SGPS09, CGMPT+08, CMBC08, CRGN07, DMLI05, DM05, GDPP08, HSMT04, HMMS09, LLL+08, LJZ+07, LS02, MRS09, PS09a, SJ+04, TCSM03, VB07, VB09, VGDSU08, XYN+06]. QMPF/QSPR [DGI+08]. QMPF/QSPR [DMLI05]. QMPF/QSPR [ZNLL07]. QMPF/QSPR [DT07, QTAIM [MGMM07b, RKA+09]. quadratic [ABBC01a, ABC01b, Bo01, HG08, Qu01, ZH09]. quadrature [CG06, DB08, GC03]. quadrilaterals [GK07]. quadrupolar [CMA+08]. quadrupole [BG03, CMJ08, EM03b, FKZ09, JBJ00, JBJ02, SSS+09, TSSG07]. quantifying [GT03]. Quantitative [Mit01, WZY04, YNZ+08, BA07, CD09, CDS09, DHW+08, DHW+09, Gra07]. quantification [GLMV09]. Quantum [AVB00, BWM+09, BS06, DM05, ECA06, ESM+06, ED04, FHR07, LBT07, MLB+00, MA05, NRK02, PM02, RM07, RON02, SC01, SS05, TLOG00, VR07, ZM+09, AGMPR+08, AGO+02, APG05, ATH+03, AGSFA05, AGSFA+05, BSJ01, BPC07, CL09, CD09, CZF07, Con02, CKW09, COL+06, DB07, DB03, DA01, DUCW+01, EB01, FC08, FA01a, FAB+00, FKFG08, FR06, FKY+05, GAIMVB01, GVATG03, Gog08, GBB07, GGLR00, GS04, HM08, HHP04, JH01, JCHS07, KSB+02, KBNH08, KJWV08, KHY00, KZRO03, KLM+09, LX07, LHP01, MBF04, MP03a, MGCA07, MKT04, MR09, MBP09, Mat03, MC06, MPF00, OYO05, OKH+02, PG04, PK07, PDS01, PV07, RP07, RSE07, RGP+07, SF07, SH07, SS00, Sau04, Sch00, SFRS01, SBB02, TCR+02, TT02, VRHR07b, Vi02, VKC09, WS05a]. quantum [WOC+03, XYN+06, XZZ04, XLZ08, ZCZ03, ZAT07, ZSK07, SB08, CGBF05, DSS03, KBL08, PF05, SCS07]. quantum-chemical [BDM03, TK05, ZWPR+04]. Quantum-connectivity [EDA04]. Quantum-regions [SB08]. quartet [MSBS01]. quartet/metal [MSBS01]. quartets [MSBS01]. quartic [SAS05]. 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 [Bof01, CPJ00, LZZC09, Lip00, Qua01, ZY01, LZZC09, ZPL07]. rack
[OCP02]. Radial [GC03, ESP04, Kan07, Knii00]. Radical
[XDS06a, AVB00, BL06, CUS00, CU01, CUS03, CXZ+09, GSB09, HIA03,
JDSW06, KOML08, KKMM04, LC07, LMK01, NSB08, O004, gThDjL+01,
WDWS06, WDS06, WDS07, WyLG+09, WLZ+07, WLL+03, XDS06b,
YLWL09, ZLLS04a, ZLLS05, ZLLS06a, ZZL+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].
Ramachandran
[SDL+09, GSB09, HHP04, PFJ+03]. Ramachandran-type [SDL+09].
Raman
[Bou01, LC09, NRKH02, OBBS05, Zero8]. RAMSES [BMRDB01].
random [CY09, CY13, CA04, HXLS09, JS07a]. randomized [LFKL00].
ranges
[CEP07, GPK05, Gg06, HGBM04, IZA06, JPCA08, KSS08, MN02,
RP07c, RLPO08, San01]. range-separated [JPCA08]. rank [RP07c]. ranked
[TBSM09]. ranking [KSM05]. Rapid
[GBA00, RSN+02, BH03, Gra07, KMH02, KCO1b, WS05a, PABK03].
Rapidly [KF02b, Zho06]. rare [LZZC09]. Ras [GC04]. rate
[Chu07, GGB07a, GGB07b, JHZ09, MGLL03, NSU+02, SLL+04b, SRFS01,
UCT+03, WLLS05, WLL+07b, WDX+02, ZP03]. rates [HG08, JIK09].
Ratio [LR06, KBB09]. Rational [Chi03, BSP06a, Ham07, VGGMM05].
rationalized [Bac05]. rattles [FS98, FS00a]. raw [RON02]. ray
[HNSW01, HN02, WKYU01]. Rb [GLRL02, GWL07, HRR05]. Re [LJKL08].
Re-examination [LJKL08]. Reaction
[CU01, JKM08, JDSW06, KKH08,
MGG06, Qua04, WCHW09, ABB01a, ABB01b, BAL+01, Bie04a, Bofo1,
BS03, CUS03, CG05, DRAS04, DRAS05, FG03, GZL02, GF08, GWM08,
Gog08, HLLS05, Hir08, HLHS05, HNT03, IN01, JHJ01, JHZ09, LMG0+09,
LMK01, LL01, LFZS04, LW04a, LDT+02a, LDT+02b, LWY+09, LLL07,
MGLL03, MG00, MS04, Mut05, NSU+02, OON01, PGG03, PGRRN03,
Pom04, PS03, PMM06, wQZsLyZ02, QZL+04, Qua01, Quo07, RSN+02, RD00,
RWHW09, RJLR06, RRo5, SLL+04a, SLL+04b, SRE08, TYN05, gThDjL+01,
TGLL07, TMBM02, UCT+03, VGB08, WLL01, WDS06, WLL+07b,
WCW08, WHG+07, XDS06a, YLZ08, YQQH09, ZLL04, ZLLS04a, ZWL+05,
ZLLS05, ZLLS06a, ZZL+07, ZLL+08, ZZL+09, dRLMS00].
reaction-diffusion
[Bie04a]. reactions
[AM07, BS03, CUS00, CFD03, Fie02,
GAIVB01, GMA04, GLH+08, GGB07a, GGB07b, HFHL06, HSWVW00,
JML07a, mJlZsLyL07, mJlZyL+08, JHZ09, KYFW07, KIM+09, LLO0,
LDC+07, MBL+00, NTH00, OY01, OY03, RNG03, Rao00a, RC04, RY09,
Rud05b, Rud05c, Sch03, Sie01, SSB07, 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]. Reassessment [DBM03]. Reassociation [DWNB01].
recently [RG08]. RECEP [KC01b]. receptor
[DLRZ09, FKA+05, FKM+06, FKM+07, GCD+08, HMK02, KBK+01,
MHL+09, SBG+09a, TFA04, TJE03, WS02b, WXC09]. receptors
[CW02, FTLV01, NHH05, YKK09]. ReCO [HT05]. Recognition
[UNHYT06, AGI+00, AGI+07, AGMP+08, BR07, CW02, DGH02,
EKB02a, EKB02b, GdSuM+07, KEB04, MSF+08, PSH08].
Reconstructing [BBP09]. reconstruction
[Ade04, GKK07, KLS02, RS08, TGD05, WGO2]. recoverin [LGB+09]. red
[McD08, SRK+00]. red- [McD08]. redesign [GLD08]. redistribution
[ZYO1]. RedMD [GSDT09]. redox [GK09]. Reduced
[BR04, BSO05, OBBS05, ABBC01a, ABBC01b, BMLV04, Bof01, CNN07,
CP08, DLD+02, EJO07, GSDT09, HP01, Qua01, RS08, WEE01].
Reduced-size [BSO05, OBBS05]. Reducing [PRSM02, SSL02, SY09].
reductase [CFERO4, CGB+09, CBC+08, DBS07, GGLR00, HLLN06, LPP06,
PCS04, PFR04a, PFR04b, TMBM02]. reduction
[CCCJ09, DBS07, DMN05, HLTLP09, LRWG03, Mck07b]. reductive [PS03].
reevaluation [Kl03]. Reference
[ZZ08, CF04, CFC+08, LZ05a, NUH02, OV03]. Refinement
[HBO9, 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, ACLD03, CFDO4, KC01a, LXW+09, LW06,
LCDA03, LCGA03, LCA03, ML00]. Relation [SM08a, DVRP+03].
relationship
[DHV+08, DHV+09, JPCA08, KWW+01, WLX+05, KKW+02]. relationships
[BA07, CDGS09, CDS09, CPUGD09, JLHF03, PSCD+09, WZY04]. Relative
[SVW+05, BLB09, CG05, MML+06, MRS+07, RSE07, ZOJ+06].
Relativistic [FHF+01, NYH02, NSO+07, SNM+06, SND02, WTKM06,
YH09, ASS+02, BHI+09, Dya02, GHLK+02, GSP06, HDMS05, HDS06,
HD06, LF02, SH02, Vao02b, VMA03, WL02, YHO7]. relax [GFS05].
relaxation [BRDC02, HS01]. relaxed [AEE+03, CA07a]. relevance
[Ano06a, MGCA07, ST06]. reliability [IB04, LKW04]. reliable
[BE06, WHF08]. remove [LZ05a]. removing [PCS04]. reordering
[TVL+03]. reorganization [FZL+06, KMM07]. repair [Pin03].
reparameterization [RFSS06]. repeat [NK01, NL08]. Repeated [KH01].
Reparameterization-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, LXZ06, LW06, RLR+04, WEE01, hYDN+08].
representations [BMLV04, LAR+03, LR06, RS08, SN00, YNW05].
representative [YLL+09, YXL+09]. reproduce [VBS09, WS05b].
reproducing [MFB04]. repulsion [COL+06, Kri09a]. repulsions [HGMB04, PBF09].
repulsive [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 [LI07, LHI09]. restraints
[BS08, HWTL03]. restricted [BdPRMAI00]. restrictions [KS09]. results
[CSD05, LKT04, PFJ+03]. Retardation [HP04]. retention [RC04].
reticulum [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 [GPSP06, JPCA08, LN01]. Rg [ZXY03, ZXY03]. RGF [HQ02].
rhenium [SBH02]. RHF [EA08, JPF+00]. rhodamine [VSW+03].
Rhodopseudomonas [IN01, OON01]. rhodopsin [CEP07, YKK09].
rhodopsin- [YKK09]. ribonuclease [SKS00, WOC+03]. Ribonucleotide
[CFER04, HLLN06, PCS04, FRR04a, PFR04b, TMBM02]. ribose [SA07].
ribosomal [SB01]. ribozymes [MMMY07]. rich [CZ05, LWK08]. Rigid
[SM03, DPRRR05, Din00, EAC06, FS08, FS00a, Ike04, Leh06, LV08, KP05].
Rigid-body [SM03, Ike04]. Ring
[ZSE08, BE09, CDPL09, DC02, DLSVY00, FJ08, RPMN07, SRE08, ZW09].
ing-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, ZZTS09]. RNA-ligand [AM06b]. RNACluster
[LOL+08]. RNase [RBWH09]. 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 [BdPRMA100, Nil09]. Rotamer [HLTLP09, GHMP03, KBLP09, LFBSK07, SMG09]. rotation [CMLS05, COMR⁺04, DHF⁺05, DBM03, HFSDB03, HK08c, LH09, LZ09a, MGLL03, OMNH08, PBF09]. Rotational [CSD05, BVW04, KBN02, TS05]. rotations [IR03]. rotors [WR07, WFR08]. 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]. RT [TYO⁺02]. Ru [ZWS⁺02]. rule [GR07]. rules [AMR04]. runs [EL07]. ruthenium [FKˇS⁺09, PHKG07]. Rydberg [PRSMV08, ZM03, dSVA⁺09].
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, FKV09, GT03, HKMS01, IS03, JW06, KH01, KM07, LWK04, Mak08, MH08b, MST⁺08, Nak02, NA06, RNO03, Rap06, SD09, SMG09, TS05, YL06, ZA07]. sandwich [JD09, RPNJ07]. sandwich-like [JD09]. sandwiched [MHS05]. sarcoplasmic [HLB09]. SARS [LZ05b]. SARS-CoV [LZ05b]. SASMIC [EA06]. Sason [Bi09]. Sb [LS08a, XB08, XK08]. Scalable [PBW⁺05, VSK⁺04, Ano05b, KKK05, Sba05, VGO⁺07]. scalar [GPSP06, KBLP09, MP03b]. scale [DMN03, JO02, KK01a, MH09, MHW04, MPF00, ME06, Nak02, NA06, RRS07, SSL02, TY02⁺0, WCF04, WS07]. scale-transformed [Nak02, NA06]. scaled [CN03, JSHG07]. scaling [AL01, AR01, Con02, FR06, GGLR00, GY06, KLM⁺09, LMJ02, OS06, RS05, SSB⁺03, SHSF05, SKDO08, SP05, TCR⁺02, ZWZ09, vGBB00, vdVGDJ00]. scanning [HMK02, MFR07, SMGE08, ZM06]. scattering [BACJCT01, Est07, HSW01, RANH03, WKYU01]. SCC [ECM⁺03]. SCC-DFTB [ECM⁺03]. SCF [JHPRSM⁺05, PFI⁺03, PVdJ00, SAM06, VZVG06]. SCH [ZZW⁺07]. scheme [Bac04, FOK⁺04, IS03, JCA⁺02, JVV09, LMV07, Maz08, MSH⁺06b, RKA⁺09, SN00, SHH07, WS05b]. schemes [Bac04, Bac05, Bac07, PRA04, SPDS01]. Schleyer [Lip00]. SCMP [FA01a]. SCMP-NDDO [FA01a]. ScO [LMCD09]. Scope [LFE06]. scoring
[BS05, GLD08, HZ06a, HZ06b, Mue01, NMAT01, OFB08, Ruv07, SBG^{+09a}, VVS07]. **SCPF** [Maz08]. **screen** [MHW04]. **screened** [RDM^{+08}, VVS07]. **screening** [DHW^{+00}, FZL^{+06}, KV00, KSM05, LFKL00, LZ05b, PRDS08, SHSF05, YOB^{+08}]. **SCRF** [CCT^{+03}]. **SCUD** [LZ05a]. **Se** [WWS07]. **SD** [WLLS05]. **SDCI** [BMB07, PRSMM02, PRSMM03]. **Se** [HKHN08, JJK^{+00}, WWS07]. **search** [AM09, BR07, BMTSC01, CSJ01, CA04, GLD08, HHG^{+09}, HXLS09, HM06, IZA06, KK01a, LFKL00, MGJAARC00, NL08, OGH05, OM04, Pu05, RHL09, Saut04, SE07, SE08, WK01, ZZ08]. **searches** [CZB07, YXL^{+09}]. **Searching** [SPT07, STC^{+08}, CvG08, Nak02, OYH09, SCC04, SYC08, YCS07]. **Second** [BC06, FS04, MO01, AGK03, JSR^{+07}, DOSG06, FO08, IN08, JSHG07, KSM05, LFKL00, LZ05b, PRRDS08, SRF05, YOB^{+08}]. **Second-order** [BMB07, Mat03, PRSMM02, ZOJ^{+06}, LSAS01]. **selective** [TCSM03, XPW09, AM06b, MHL^{+09}]. **selectivity** [BS06b, GLRL02, OO08, ZZvRSC08]. **Self** [ZA07, BA08, BWI^{+02}, ECM^{+03}, NUH02, NTH09, NL08, SH07, TKB03, VTT^{+08}, WM04, XL02]. **self-associative** [NL08]. **self-consistent** [BWI^{+02}, NUH02, VTT^{+08}, WM04, XL02]. **self-contained** [SH07]. **self-interaction** [NTH09, TKB03]. **Self-organizing** [ZA07, BA08]. **semi** [BBHD04, UKN04, ZNLL07]. **semi-** [UKN04]. **semi-empirical** [ZL05a]. **semi-implicit** [BBHD04]. **Semiautomatic** [PRJ02]. **semibullvalenes** [HS05c]. **sensor** [BBG^{+04}]. **sensors** [EA06]. **sensitization** [SS05c]. **sensitized** [KS05c]. **sensitivities** [HL04]. **sensitivities** [Sh04]. **sensitization** [SS05c]. **sensors** [BBG^{+04}]. **Separable** [EA06]. **separated** [JP08, MLL06, S06]. **separating** [CN03]. **separation** [FBG06]. **sequence** [AM06b, CCWH02, CKR08, CLZX09, Dya02, JIK09, LXZ06, LSW^{+01}, PRJ02, WHH^{+06}, ZLY07]. **sequence-dependent** [LW^{+01}]. **sequence-specific** [PRJ02]. **sequences** [CP09, DLW06, DLWV07, Der00, JIK09, LW04b, LD05b, LW06, MCF07, PP08a, hYDN^{+08}]. **sequential** [TT05, ZGZX07]. **SER** [JP08]. **serially** [KMA^{+07}]. **series** [CC07, KMH02, PDS01]. **serinamide** [PFC03]. **serine** [OB09]. **serotonin** [HLC09]. **serve** [Mck07a]. **set**
set-up [GGT08]. sets [BY06, BSOB05, CRS05, Cu04, EA08, EdlVR+03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NSO+07, OBBS05, OVMV04, RLA01, RLRE01, RLER07, SNM+06, VB03, WTKM06, Wei08]. setting [HP04]. setup [ZAT07]. several [KS05b, XLT07]. sevoflurane [TZX01a, TZX01b]. SG [CG06]. SG-0 [CG06]. SGB [GZL02]. SGB/NP [GZL02]. SH [Mas01b, MGLL03, Mui05, SSS+09, WLLS05]. SH/ [SSS+09]. SH3 [IGNH03]. Shaik [Bic09]. shake [KFD06, BL09, FS98, FS00a, KvGH01]. shake-up [KFD06]. Sham [Bou00, RRS07, SH02]. Shannon [LM03]. shape [BR07, PRDS08, WM06]. shape-based [PRDS08]. shaped [LWW+06]. Shapelets [PRDS08]. shapes [BR07, KS02a]. shaping [HJCP01]. shared [Sim07]. sharing [BR07, RS07a, RS07b]. SHARPEN [LMH+09]. Shaw [Ano05b]. sheet [KF03, PP08a]. sheets [LLW02, PGC05]. shell [DSB+02, FS02, FO08, HB09, PRMM03]. shielding [CDL06, CDPL09, HWFN01, MC06, PFC03, WZXY07, ZPL07, ZXY08, ZLD09]. shift [Dr00, HP05, LFZS04, MA05, RG02, WPS02, XZ04, ZFL+05]. shifted [McD08]. shifting [CPFL02, HRG07]. shifts [CPDZH08, FVB08, FH+01, FO04, HWFN01, HLLN06, Kle03, KKS04, LFS+07, LKA01, VBS09, WFHP01, WHP02, WZXY07]. SHOP [YXC+07]. SHOP-type [YXC+07]. Short [TYN05, GP05, HGMB04, IKYM09]. short-range [GP05, HGMB04]. Short-time [TYN05]. shorter [MST+08]. Si [BSB05, TK08, WZZ+09, YHD+06, CJS+03, SURG06, WL09b]. sialic [UNHYT06]. SIBFA [PWHF+03, PWHF+04, ROG00]. SIBFA-LF [PWHF+03, PWHF+04]. side [DLHC06, ENM+04, GT03, HFHL06, JF+00, KG02, LL01, MT03, MMLC05, PFC03, SMG09, VM02, XLT07, ZM06]. side-chain [ENM+04, GT03, JF+00, KG02, MT03, PFC03]. sieve [PHH+08]. sieves [LMV07]. SiF [LAT05]. sigma [JFG04, KMM07]. signatropic [LLKC06, LFS+07]. SiH [ZZL+09]. silastannation [WCHW09]. SiLi [XF06, HX08]. silica [SDCG02]. siliceous [LST08, LTV08]. silico [LLW+09, MWH04, PHR+05]. silicon [BSB05, HX08, KZV+05, KS01b, LB08, NBJ04, ZLJS03]. silsesquioxanes [JW00]. silyl [MGG06]. silylenoid [XFF06]. SiMe [XFF06]. similar [BR07]. similarities [HPP00]. Similarity [Leh06, LhWX07, ARL01, BPCD07, COS01, Con02, HM08, MBH+02, PDS01, RSS09, YN05, hYDN+08, ZZTS09, dGWH01]. similarity-based [RSS09]. similarity/dissimilarity [hYDN+08]. Simple [MO01, Ste04, ACLD03, Bac04, BLMS08, GRO+03, GDV03, Gon07, ILB03, IT03, KS02a, LLW+09, MCF05, SF05, BG00]. simplex [DV02, MCF05]. simplex-annealing [MCF05]. simplified [OYH05, WOC+03]. simulate
simulated
[ADM+06, AB08, CCP04, HPP00, RLP08, WM06, WG02]. Simulating
[Fie02]. Simulation [FBGD06, WWL+09, BBHD04, BVW04, BG07,
BBM+09, CCD+05, CV09, CHB+05, Dra00, EA06, EMP07, FHR07,
FEV+09, FPN+05, GS02, GJK00, HN02, HLB09, ITS05, IM06, IKYM09,
JO02, JGVF05, KSY+00, KB09, KEM08, KPR04, Kri09b, LMCD09,
LEV+09, MLG04, MMMY07, MVL+05, MLCD01, MST+09, ON07, OBT09,
Pin01, PHH+08, SO07, SL06, SDL07, TYN05, VHRR07b, WEE01, XKG
+05, YAC¸ +02, YTH+07, ZALMG03, ZWTP+08, ZL09b, ZSK07, OBBS05].

Simulations [FCP+05, MZL08, ATMK03, Ano06c, BWE05, BRDC02, Bie04b, BSJ01,
CLP09, CLWL09, CLC09, CCSJ00, CF06, CPC+00, CEP07, CMD+04,
CBH+03, DHF+05, DLRZ09, DFG09, Der00, DSS03, DWC+03, ESM06,
FGR07, FG02, FCP+04a, FAB+00, FC06, FKZ09, GL04a, GLP08, GWM08,
GH07, GS03, Gon07, Haf08, HB09, HGMB04, HHHS01, HH04, HM02, HPL03,
Hin00, HFS03, HTKGO8, HTSR04, HTN03, HMD06, IC08, JNV08, JCL05,
JZD+09, KMKH02, KFZ03, KM00, KK05, KAK+09, KvGH01, KH06, Kr08,
Kr03, KBN02, LML+00, LSO04, LGB+09, LM03, LPB03, MB00, MFB04,
MN02, MABM09, MBC08, MO09, MG00, NK01, NL07, Ni09, OO06, OR05,
PRPK05, PHJ+08, PB04, PMB04, FK04, PB02, PNG08, RPMP03, RSER09,
RMHK03, SK09, SDL+09, Sch04, SBRG09a, SWR06, SR09, SDM02, VCM01].
simulations [VHRR07a, VP09, WL09a, WCF04, WZW+06, XLZ08, YNZ+08,
YGLvG06, ZCS04, ZSC05, ZGFI01, ZWS+09, ZW09, ZSK07]. simulator
[JGVF05, KIM+09, MS04, SO07]. simultaneous [DDVD09]. Singh
[JVVK09]. Single [OV03, BG07, CV09, HSF08, IT03, IKYM09, LFZS04,
WTKM06, XXL+09, ZZvRSC08, Mak08]. single-family [WTKM06].

Single-nucleotide [Mak08]. single-sphere [LFZS04]. Single-step [OV03],
single-walled [XWL+09, ZZvRSC08]. singles [IN08, WKY01, DSA+09].
singlet [BLO+02, CZ05, CG08, FG03, LS08a, OSA06]. singlet-dioxygen
[BLO+02]. singly [HHWG08]. Singular [FPG+06, TBSM09]. Sir [An04a].

Site [CJW+09, LLL07, AG00, CRF06, CFS+09, CF04, CIFC+08, FPN+05,
GJK00, GS04, HFS+07, HYR06, KSK00, KEB04, KZRO03, MDA08, NL07,
NLL+09, PNN06, SS05, SPT+03, SFR07, TDH06, XLZ08]. sites [APG05,
BSP06b, BSM04, CLXC02, CLS+09, DV02, FPN+05, FSS00, GDV03,
HM02, HNO2, HLT+05, MHJS06, PPAX01, SEK09, SLK+09, Tie09, Wou00].
six [GJK00, NL07]. six-site [GJK00, NL07]. sixth [CGB+09]. sizable
[CAG07]. size [BSOB05, EL09, HLTL09, KS02a, KH06, NK06, OBBS05, OV03, YAÇ+02].
sized [SHH07]. Slater
[CVVB04, EdlVR+03, GC02, KDG+09, RLER04a, VB03]. Slater-type
[CVVB04, EdlVR+03, GC02, KDG+09, VB03]. slave [FR06]. small
[CN03, Che01, CG06, FM00, IME02, IO08, JARM02, Kvh01, Lei06, LZA02,
Oos09, PO03, PBZ00, PDS01, RRS09, RZWS07, SHH07, TYY+02, Van02a,
WS02b, ZP03, ZOJ+06, ZX09]. small- [SHH07]. smallest [SRS07]. SMART
SMART-based. smooth [GP01, KSY+00, PZS04]. smooth-particle [KSY+00]. smooth-permittivity [PZS04]. smoothed [LV08]. smoothing [HPPO0, ILB03, WS02a]. snapshot [YNZ+08]. SnCl [RD00]. sodium [FL07, MH05b, YSJ09]. SODOCK [CLH+07]. Soft [vChHuY08, ASDP+06, TLKT00, TJE03, TGGP+00]. soft-core [TLKT00, TJE03]. Software [Ano04b, BACJCT01, DvL01, Gly06, JVK09, CHB+05, GBDP05, KBA+04, Issh02, KCK+08, SK05]. solid-state [CMA+08]. solids [vDSSvA04, JB04]. SODOCK [CLH+07]. Soft [yCkHmY08, ASDP+06, TLKT00, TJE03, TGGP+00]. soft-core [TLKT00, TJE03]. Software [Ano04b, BACJCT01, DvL01, Gly06, JVK09, CHB+05, GBDP05, KBA+04, Issh02, KCK+08, SK05]. solid-state [CMA+08]. solids [vDSSvA04, JB04]. Solids [vDSSvA04, JB04]. solubilities [SH07]. solubility [BBG+04, EDAJ04, KEH+02, LLW+09]. solute [BRLS08, BRLS12, FCP+05, LFZS04, MR04, YL09, ZSK07]. solutes [BLL+06, HMSM06]. solution [ABWT09, BH00, BP07, BISB02, CP00, CCK01, CRSB03, DA01, EK06, ELK+09, FHR+06, FG02, GAMA04, HHJ03, HMWC03, HSVNRN01, HRR05, HBW00, HBW01, HDO+02, KPR04, Kri09b, KBN02, LRI+02, LXF08, LMF06, MB00, MH08b, PDP02, PTC01, PHRR+08, RN03, RR+08, SH09, SATO04, SB02, TDH06, Vas02, VBS09, YH06]. solution-phase [TDH06]. solutions [Blo04, CP01, Loe03, PK04, VP09, XZ04, XZ05, ZWP08, LR+03b]. solvated [HTSR04, HRR05, KHY00, QSS01, RSP03, BSC+01]. Solvation [COL01, HHP+04, WB04a, WB04b, WB05, WD04, BCIB05, CRSB03, CCT+03, COL+06, DV02, DWH+04, FOL+04, FBL00, FZL+06, GS02, GS03, GP01, GWS+02, HC08, HLMR06, IV04, IvSV06, KIM+09, LF04, LFZS04, LS08b, MGLO03, OVMV04, PZS04, PPYS08, RSE07, RP04, Sch00, SDL07, VM02, VP09, XL02, ZFL+05, ZFL+05]. solvation-effect [SDL07]. solvatochromatic [XZ04]. solve [KvGH01, XOW+00, Zh06]. Solvent [BA03, BA04b, SMADV00, ZP03, ZGFL01, AG03, BH00, BBHD04, BMLV04, BRLS08, BRLS12, ENM+04, FEV01, FC06, GZL02, GL04a, GP06, GB04, HHS+05, HN02, JS07a, JZD+09, KIFK07, Kro03, KKS04, Lab08, LRI+02, LFSBK07, LS04, LL01, LFR+04, MBC08, MM07, MCM04, MS01, RR+08, RP07d, SBLK01, STSF02, SHSF05, SL06, TJE03, TSMNG01, Tot+04, VBGL+00, WB04a, WB04b, WB05, WWL+09, YTY07, YXZ+04, YL09, ZXL09, BA04a, FZL+06]. solvent-accessible [BH00, BMLV04, HHS+05, TSMNG01]. solvents [GS03, IT03, THHN01]. Solving [FS00b, Hf05b, BF04, CCL06, CF04, LMJ02, SAT004]. Some [VE09, FMPS08, JARM02, KCL06, McD08, Rao00a, Sch03, WL04, YLL+09, CMA+08]. sometimes [BE06]. Song [JW12]. Sons [Bie09, Lip00]. source [CSV+07, GCB03]. soybean [TGLL07]. sp [NYK+09]. space [Bie04a, BMTC01, CSJ01, Cy08, CT+08, CZA03, GM03, HXLS09, JO02, KFO8, LCKL05, LJL08, Nak02, NA06, OFIK09, PFR+05, PBF07, PBF09, PRSMM02, QNF09, Sch04, THHN01, Van02a, YL06]. spaces [JHP+05, PRSMM02, PR+07, PRT+08, RSS09]. spacing [ZZvRSC08]. spanning [SN00]. Sparkle [FSG05]. Sparkle/AM1 [FRS05]. Sparse [SSB+03, AGSFAL05, LEK07, RS05, RRS07]. sparsity [JSHG07]. spatial
specialized [Hof05], species [CFC+08, DR09, GHLK+02, HBM06, KZY09, WG02, YIN03, LMGR05].

Species [FAR02, LR03a, BS08, HLTh+05, Pin01, PRJ02, SFRS01, TGLL07, TST+08, UHN09, WCF04].

specificities [PB06].

specific [FAR02, LR03a, BS08, HLTh+05, Pin01, PRJ02, SFRS01, TGLL07, TST+08, UHN09, WCF04].

specification [CJW+09, DLRZ09, LLL07].

spectroscopic [Ano06a, FCW06, KCL00, ST06].

spectrometric [KZW+05].

spectra [Bac09, BACJCT01, CNN07, CG08, Gor01, HKHN08, JARM02, KŠB09, KFD06, LDL+09, MLCD01, NRKH02, OBBS05, OKE+02, ŠBL05, SN06, TDI06, WM01, YXZ+04, ZGX06, ZWT+08, dGWH01].

Spectral [II02, CVR08, GdSuM+07, LFZS04, NINAT+07, NAT07, SMKM00, WG02, ZSK07].

spectrophotometric [KZW+05].

spectroscopy [ACM+06, RDM+08, VDM06, WMRW+01, ZPL07].

speeding [KVF+07].

Speed up [BYQS03].

sphere [HdMdS05, HdS06, HD06, LFZS04, SFR07].

spherical [BCIB05, ZFL+05].

spheriphane [CS01].

SPICKER [ZS04].

Spin [Duk01, HYR06, KTM02, LXSF08, Van02b, ACM+06, BB08, BACJCT01, CR08, CR09a, DXW08, DPT03, DF04, JSHG07, KRM+02, KRLD09, KK08c, LB08, Mck07a, Mck07b, VCM01].

spin-crossover [KRLD09].

spin-label [VCM01].

Spin-orbit [KTM02, LXSF08, CR08, CR09a, DXW08, KRM+02, LB08].

Spinor [PV03].

spins [JD09].

Spiro [HELM09].

spiroquinazolinones [DD08].

spline [ALKH04].

splines [GL04b].

split [EA08].

split-valence [EA08].

splitting [PSD00].

splittings [HLLN06, SFRS01].

Spontaneous [Sza08].

square [CSB08, LLZL09, Nil09].

square-planar [CSB08].

squares [CSD05, Gol09].

Sr [WD08, SCP08, XB08].

Sr-doped [SCP08].

Src [O008].

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, ZXY09, ZOJ+06, ZM06].

Stabilization [EBDPM00, HYA02].

stabilized [HSF08].

stabilizing [GZ07].

Stable [HDO+02, GDPCPU07, KYFW07, KZY09, KAS+07, Ko04, LMO09, PP08a, PZS04, STC+08].

stable/nonstable [GDPCPU07].

stacked [RRA08, SB08].

stacking [CM09, DDBP09, HWT03, KKY01, WRP+06].

standard [ASDP+06, CG06, FBDG06, KOFF09, LFSB03a, LFSB03b, SSS+09, SL04].

standing [KDG+09].

staphylococcal [JS07a].

Starting [VZVG06, BWI+02].

state [Ang09, BBI+09, CWY09, CFS+08, CHA+07, Chu07, CAG07, CMA+08, HM01, HNWF07, HNWF12, Hir08, HP05, IEME02, JHZ09, 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, Bof01, Bon01, CWY09, CNN07, DHM+03, DF04, EL07, FCW06, FDSA00, HFS+07, HYR06, HZ09, IR03, KUB07, LS08a, LWX07, LB08, MW09, MLCD01, NBTN04a].
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 [HFSD03, PYEA03, DW08, EC06, Kob03, RK05, SBJ08].

statistical-thermodynamic [RK05]. step [BYQS03, BCP03, DLW06, KM00, KH06, MK02, Mck07b, OV03, Oos09, ZWZ09]. step/particle [BYQS03]. stepwise [LLKC06, LFS+07, NSB08]. Stereodynamics [CMLS05]. Stereoelectronic [SK09]. Statistical-thermodynamic [RK05].

step [BYQS03, BCP03, DLW06, KM00, KH06, MK02, Mck07b, OV03, Oos09, ZWZ09]. step/particle [BYQS03]. stepwise [LLKC06, LFS+07, NSB08]. Stereodynamics [CMLS05]. Stereoelectronic [SK09]. Statistical-thermodynamic [RK05].

stranded [AZM03].

Strategies [DBS08, LJS05, YL09, EKB02a, EKB02b, KEO4, Vis02]. strategy [BME05, CZA03, LLL+08, MCF07, RI08, SMGE08, Wan09, WS02a].

streamlining [VGB08]. strength [DMJV05, Fau01, KEM08, Sau04, AM09, CSJ01, DHP+05, GdSuM+07, MKT04, ZZ08].

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

stratonium [RD06]. Structural [CZF07, EM03a, Kri09b, LWLS07, LFR07, MS03, BCP03, CRK08, CLF+09, ECM+03, GZ07, HYA02, HHP04, KZY09, Kar06, KPK06, LL07, LJS05, NAT07, OFK09, PK04, QHL09, SLC+09, SVV+08, SRB06, XSS06, XLC08, ZLS05, ZWP08, CA07b]. structurally [AGMPRG+08].

Structure [BMTSC01, CDL06, HHWG08, HRR05, HS07b, ITS05, KCL06, KPR04, MN02, PGCG05, PLC08, PHRR08, RG08, SG07a, AJ03, AGFS+05, BED02, BS01, BAH+02, BA07, CLO03, CZB07, CDS09, CDS09, CMaGL+04, CJS+03, CN05, CLA+00, CPUG09, CSV+07, DP03, DHW+08, DHW+09, Fan01, FL07, FLOD07, FCP+04a, FL08, FLK+07, GBL+05, GTC06, GGGGL05, GdAc+07, HHJ03, HEP+02, HNO2, HP05, ILRK09, JCA+02, JLHF03, KP05, KFN08, KHY00, KOF09, KBK+01, KBL08, KIFK07, KWK+00, KGD06, LEK07, LJKL08, Lee09, LLP06, LZA02, LZ05a, LCSZ09, LW06, LOL+08, LYH+08, LDK+09, LR03b, Loe03, LLL07, MOP+07, MM00, MLL08a, MM02, NK01, NYH02, NCO+05, OS08, PDP02, PSCD+09, PJB+07, PPM05, PRJ02, PF06, QB05, RPNJ07, RI07, RS05, RSS+03, SSB+04, SB01, SCP08, TD08, TT01].

structure [TGD05, Van02a, VHRR07b, WZ04, WMRW+01, WD08, WS07, XYZ04, YXL+09, ZZY07, ZZS+07, ZZY08, ZLD09, ZX08, vDSSvA04, vEMK01, vEO1, RRCA08]. Structure-based [BMTSC01, HS07b, KBB+01].

Structure-breaking [HRR05, VHRR07b]. structure-properties [CDG09, CDS09]. structure-property [JLHF03, PSCD+09]. structured [DC02]. Structures [AB00, CTFC08,HXD08, KS05a, PCMG09, RSSKB03,
[SK05, SLRC01, SVV+08, SMV+09, SSBE06, TBG00, gThDjL+01, TD08, TT02, UNHYT06, UNM+01, UM03, VHR07b, WZY04, WC09, WMRW+01, WD04, WLPX+05, WLLS05, WDS06, WDXS06, WDZS07, WLL+07b, WCW08, WWT08, WZ+09, WM04, WOC+03, WD08, Won09, WDX+02, WRRB03, WC08, WJX+08, XYN+06, XZ08, XDS06a, XFFF06, XXWC08, XKG+05, XPW09, YT03, YT04, YTY07, YXZ+04, YDS06, YXC+07, YLZ08, YLM+08, YQQH09, YHD+06, ZP03, ZPL07, ZZZL04, ZLS+04b, ZLLS05, ZLLS06a, ZLLS06b, ZZW+07, ZZL+09, ZHL08, ZYW+09, ZNLL07, ZX08, ZTP+08, ZL07, dSVA+09, dRLMS00, LSAS01, NBJ04].

[AGI+00, AGI+07, dVB01].

[AGI+00, AGI+07, dVB01].

[Ama02a, Ama02b, XPW09].

[FS00b, Har04].

[CCP04].

[ATH+03].

[RK05].

[Substituent][JWB05, Lee09, PWFS01, BPC01, HMMS09].

[Substituents][PSF+08].

[Substituted][AVB00, BE06, BE07, HM08, HWGB01, LST08, MMY+07, MRS09, OSA06, PB05, RF09, TTB01b, WyLG+09, WW04, YDWS06, WFHP01].

[Substitution][ZZS+07, BS05, JT06, LFBSK07, SOOF05, SS07, ZWS+02].

[Substitutional][FSS00].

[Substitutions][CM09].

[Substrate][BMTFR08, LCC09].

[Subtype][FTLV01].

[Subunit][OOO1].

[Successful][CLA+00].

[Successive][IR03].

[Sufficiency][LLW+09].

[Sugiura][TKN+08].

[Suitability][FMSA06].

[Sufluor][SL.04a].

[Sulfate][ZZW09].

[Sulfation][CLS+09].

[Sulfide][DLR+08, GGGLL05].

[Sulfonylurea][XYN+06].

[Sulfoxide][CFD04, EBDPM00].

[Sulfur][BT00, CGB+09, SO06, SV06, TTB01a, WS05b, FNP+06].

[Sulfuryl][CQ04].

[Sum][Bou01, SG01, UKN04].

[Sum-over-states][Bou01].

[Summation][Ami00, San01, SG01].

[Superatoms][LWW+06].

[Supercells][EL.09].

[Supercomputers][MOP+07].

[Superconducting][MDI04].

[Supercritical][HTN03].

[Superexchange][WL00].

[Superimposition][ZA07].

[Superlinear][FR06].

[Supermolecule][BA03, BA04a, vDSSvA04].

[Superoxide][PPM06, RJLR06].

[Superposition][COS01, CSD05, GRDC01, GCD04, IO08, Mas04, VKP+08, VZVG06].

[Supershort][XWI+09].

[Support][CLXC02, LIZ+07, YM04, CLS+09, HL08, LCC09, QHL09, Mui05].

[Supported][GTC06, KEM08, SD09].

[Suppressants][LDC+07].

[Supramolecular][AM07, CMLwGL+04, Won09].

[Surface][ABB01a, ABC01b, BMLV04, BL06, Bof01, BHH+09, CF06, DLD+02, DR09, EBL+08, GLL02, GCD+08, GB04, HHS+05, HG08, JBG08, KLM+04, KCK+08, Lab08, LMK01, LFBSK07, LJO4, MG06, NK06, Pan07, PHJ+08, PFJ+03, PTC01, Qua01, RSN+02, RP07d, SURG06, Sau04, SMGE08, SL06, SDL07, Sza08, TSMN01, TRS02, VP02, YHD+06, YJF06, ZCS04, ZSC05, ZCL09, ZGFL01, ZBS03, ZXYF09, ZGXX06, EKB02b].

[Surface-adsorbed][DR09].

[Surface-doping][JBG08].

[Surface-generalized][YJF06].

[Surfaces]
surrogate [Mck07a].

surrounding [KGL07, Yos02].
survey [HS07a].

SuSi [CA04].

SVD [CSD05, WG02].

SVM [CSD05, WG02].

SVM(TM) [YMT04].

swarm [CZB07, LJZ07, SJJ04, CLH07].

switch [SF07].

switching [GG09].

symmetric [AT02].

symmetrically [Lai07].

Symmetry [PDC08, PCA08, BB08, CAGR08, FCP04b, LWX07, SZW05, LWL07, PT01].

symmetry-adapted [FCP04b].

Symmetry-driven [PV03].

Symmetry-generation [Ell07].

Synergistic [GS08].

syngas [YQQH09].

synthase [BBSS06].

synthesis [HLC09, PHR05, WLL01].

synthetic [NHH05, WG02].

system [BL00, HELM09, HRBKB03, IS03, KLY03, LHJ06, LCGA03, LTDTS07, MM03, PHG04, PRSM03, Rud05a, YOB08, ZAT07].

Systematic [AST06, CS03, KWHH07, Kob03, LSAS01, MV06, PK04, PG04, RS05, WM04, WZXY07, ZXY08, Dya02, PWFS01, PV07, SYY03, WK01, EA06, LHM09].

systems [AS00, BHW00, BP01, BME05, BGJ01a, BWI02, CN03, CG06, CvG08, CCK01, CMGDAC07, DXW08, DRMD03, Don08, DK01, EGSG00, Ell07, FZL07, Fau01, GLMV09, HT03, JCA02, JTR05, JG03, KSS08, KKC05, KAK09, KBL08, Kle02, Kle03, Kri09a, LMJ02, LC09, LLL03, LDG02, MMLC05, MKGA06, MTB09, MM07, MS01, Oos09, RLD09, RSN02, Rud05b, Rud05c, SRS07, SS00, SY03, SVW05, ST01, TH02, TT08, WWL09, WH03, YCXY03, YZ04, vdVGDJ00].

T [BBI09, Lu09, PFJ03, ZKZ07, DLD02, Ike04, KVS06].

T-cell [KVS06].

table [Kan07, Nil09, SRB06].

tableaux [SN00].

tables [ARL01].

tabu [MGJAARC00, SE07, SE08].

tailoring [BG03, KKG09].

taking [SN06].

TaN [ZHMW09].

tandem [UNHYT06].

tantalum [Tie09].

target [FM00].

tautomer [LS08b].

tautomerism [YXZ04].

tautomerization [BA03, BA04a, BA04b].

tautomers [HHWG08, PG04].

TCNE [GYMM07, TD08].

tCONCOORD [SD09].

tCONCOORD-GUI [SD09].

tD [CHA07, SBI08].

t-DFT [CHA07, SBI08].

tDDFT [SL04].

tDHF [QCK01, QCK02].

tau [HKHN08, WWS07, HFWN01].

technique [COS01, GKH05, KLM09, SAT004, TS05].

Techniques [Woo01, You11, AM06b, DC02, FSM09, KH05, PAT09, PDS01, VE09, WSM09, vGGB00].

Teller [Kri08, VDM06].

temperature

[FGR07, JS07a, KT02, KGD06, MN02, TD08, KX08].

temperatures [KK01b, TK08, WHH06].

tempered [BBP09, CVVB04].

tempering [SPT07].

templated [ST04].

tensor [BZP09, BAA07, RI07].

tensors [CDL06, KRM02, ZLD09].

term [JCHS07, SP05].

terminal [KK01a].

Terms [Duk01, BMIV04, HP01, LAR03, RP07a, YZ06].

ternary [Don08, MM07].

territory [Sha07].

tert [Bac09].

tertiary [CML05, PRJ02, PF06, SO07].

tessellation [LJ04, PTC01].

tessellationless [Pom04].

test [BCF09, BUMCMRL00, BLN01, BE06].
CF04, FMPS08, KTM02, SB108, SM03]. Testing [CMaGL+04, BG03, PZS04, WWC+04, WWC+05]. tests [KSB+02, NGTB03]. tetraammonium [CW02]. tetraazanaphthalenes [CdML06]. tetrachloride [DMN05]. tetracoordinate [MMRVH07, SRS07, Wan09]. tetracyanoethylene [LM02]. tetrahydroimidazo [CdML06]. tetracyanoethylene-contained [LM02]. tetrahydroxouranylate [IvSV06]. tetramer [RRCA08]. Tetrazine [JW12, SLHW09]. Tetrazino-Tetrazine-Tetraoxide [JW12, SLHW09]. tetrazole [dSVA+09]. TGSA [GRCD01, GCD04]. TGSA-Flex [GCD04]. Their [NSO+07]. their [Bac04, Bac05, 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, Bior03, BS03, CNN07, CFD03, CFD04, CG08, COMR+04, FJ08, FL07, FDSA00, GYCZ04, GLH+08, HLLS05, HS00, IGL07, ILK09, mJZyL+08, JW12, KYFW07, KZY09, KSN01, KS05c, LS08a, LH02, LWX07, LDY+08, LLW02, LTD+02a, LTD+02b, LYZ+08, LMRVFH+09, MMLC05, MCK05, MBM+00, NBTN04b, OCP02, OKE+02, PFR04b, wQZsLyZ02, RTG00, RZSW07, PLL+04b, SFR07, ST06, TKS+01, TJM+03, gThDjL+01, VS08, WLL01, WWL09, WDS06, WDX06, WDS06, WLL05, WLL05, WCL05, WJX+08, XFF06, XKKL03, YTY07, YIN03, YFR05, YLW+08, YQQH09, YLWL09, YHD+06, ZLLS04b, ZLLS04a, ZLLS05, ZLLS06a, ZLLS06b, ZZ+07, ZZL+08, ZZL+09, ZWW09, ZX03, ZL07, BGC+09, CN05, DL+08, GX09, Ham07, HRBKB03, HLMR06, Kan07, KKKMS04, LC07, LD05a, Lee09, LL01, LLK06, LB08, MM02, MD10, NT2H00, NBS08, Nye07, OON01, PGRRNG03, PC00, PSS07]. Theoretical [RAGL09a, RAGL09b, RRS06, RP04, RJLR06, SLHW09, SMV+09, UNHYT06, WLZ+07, WSM+08, Wou00, XXW08, YXZ+04, ZL05, dRLM09, Li01, NBTO4a, RD00, UNM+01, ZPL07, ZLD09]. theoretically [WS02b]. theories [JH09]. Theory [BBC+05, SH08, WM12, ALT06, ASDP+06, ASY01, BC06, CWY09, CFK08, CR08, Ch07, CKW09, CPML08a, Cu08, CGSdST06, DPM09, JRS+07, EL07, EKB02a, FCW06, FZL07, FG02, FI+07, FLG00, FS04, FLK+07, FZL+06, GM01, G03, G04, Ha08, HM04, HS07a, Hol05, ION07, ION08, IN08, JCHS07, KSS08, KWK+01, KWK+02, KK08c, KZW+05, Kt07, LMB08, LF04, LFZ04, LMGR05, LF02, LLZL09, LL+09, Lu09, MGMM07a, Mat03, MW09, MA09, MH08b, ML00, NY02, NU02, NTH09, OFIK09, OKE+02, PFJ+03, PS+08, PU09, PA05, Qr+08, RB01, RDM+08, RZWS07, SH07, SH02, SZT08, SSMW09, SSB07, SW06, TST+08, Tru07, TKN+08, T05, WR+06, W07, WZY04, WMRW+01, W03,
WCHW09, WL00, WCFH02, WNH03, WCL05, XYN+06, XB08, XL02, XPW09, YCX03, YH09, YYW07, YLL+09, ZL04, ZH08, Zho06. theory [ZFL+05, dOMSL01, vGGB00, vLBBR12, Blo04, BE09, CGMTPT+08, GGI07a, PFBO5, PMC+08, SG07b, ZSC05, Bic09]. theory-based [XL02].

Theozyme [UTH+03]. there [KT02], thermal [LZZC09, LLKC06, Lu09, SFRS01, WXK08]. Thermally [ZALMG03]. Thermodynamically [BT00]. thermochemistry [LLXS02, ZXL+04]. Thermodynamic [NA06, WR07, WFR08, ZWP08, Blo04, BZL05, KS05b, KK01b, LC06, LLZL09, RK05, SY09]. Thermodynamical [KZY09].

Thermodynamics [UNM+01, HFS03, JMD+02, MH09, NSU+02, PCMG09]. Thermoelectric [WK08].

Theriostats [MZL08]. these [LL00]. Thiamin [LS08b]. Thiazole [XKG+05]. Thio [MMMY07, TTBO1b]. Thio-substituted [MMMY07, TTBO1b]. Thioacetalization [RUPH06]. Thioamide [LKJ+04]. Thioamide-containing [LKJ+04]. Thioether [SFR07].

Thiolate [DMN05, SGD06]. Thiomandelate [APG05]. Thiopeptides [TTBO1a, TTBO1b]. Thiophene [KTM02, PSF+08, RRCA08]. Thiophosphoryl [ZJM+07]. Thioredoxin [CFR06, CFS+09]. Thiouracil [LMGO+09]. Third [BGJ01b, Gri03, JGH00, KGN07, LK04, RRP+01, YTH01]. Third-order [Gri03]. Third-row [BGJ01b, JGH00, LK04, RRP+01, YTH01]. Thomas [Kri09a]. Thorium [AB00]. Threading [BS08]. Three [BY06, BP01, Bie04a, BB08, BGC+09, CV09, DW+07, FLOD07, GDV03, HK08c, KBL09, Lai07, MP03a, MVL06, SHB05, Wan09]. Three-body [FII+07]. Three-bond [KBL09]. Three-center [Lai07]. Three-coordinate [BGC+09]. Three-dimensional [BP01, MP03a, MVL06, SHB05, Wan09]. Three-point [Bie04a]. Threshold [Mei02]. Thymidine [LBG08]. Thymine [KKMMS04, MHS05, NBTN04a, NBTN04b, Pin01]. Thymine- [MHS05].

TIBO [AJNG01, SGPS09]. TiCl [UNM+01]. Tight [ECM+03, HNWF07, HNWF12, WM04, XL02]. Tight-binding [HNWF07, HNWF12, WM04, XL02]. Tilt [LH09]. TIM [AGK03, LD05a].

Time [Bac09, CP08, Gog08, Kol04, LD+09, Whe08, ZH08, BYQS03, CFK08, CPC+09, DF06, FCW06, HNWF07, HNWF12, HS01, ION07, KMH02, KM00, KH06, MW09, NTH09, PK05, PSF+08, TYN05, TST+08, TKN+08, YH07, ZWZ09, ZM03, vGGB00]. Time-averaged [CP08]. Time-dependent [Bac09, Gog08, LD+09, Whe08, ZH08, CFK08, FCW06, HNWF07, HNWF12, HS01, ION07, MW09, NTH09, PSF+08, TST+08, TKN+08, YH07, ZM03, vGGB00]. Time-frequency [DF06].

Time-reversible [Kol04]. Time-step [KM00]. Times [DDVD09]. Timescale [MST+08]. TiN [JD09]. TINKER[TM] [Sto05]. TiO [FHRR07]. TiP4P [HPL03, THHN01]. Tires [LMGR06]. Titanium [UNM+01]. Tl [VHRR07b, VHR07a]. TIN [ZL09b]. TIX [ZL09b]. Tm [BM00, GM01]. TMPyP [AZM03]. Toluene [GCCVB00]. Tomography [RGG08]. Tool
transformational [CN03], transformations [WSM+09], transformed [Nak02, NA06, vDSSvA04]. Transition
[FKRE08, LMGR06, TH02, ABYM08, ABBC01a, ABBC01b, Ano06a, Bac05, BP03, BS06, Bofo1, BRV+07, BM00, BGJ01b, CWWS07, Chua07, DLW06, Dib05, EL07, GH07, GM01, Hol05, JHZ09, KRM+02, LW07, LD05a, LH02, LGB+09, LW09, LK03, LK04, NR04, PYCD03, Qua01, Qua07, RRFC+03, SK09, Szo08, ST06, TKS+01, WB07, WL09b, YTH01, ZALMG03].

transmembrane [GAS04, YMT04], transport
[Ara04, CM09, FCP+04a, FCP+05, KK08c]. treating [MA09]. treatment
[BCF+09, BZL05, CLA+00, CBH+03, HC08, HHBH00, IB04, JB04, KS05b, KCL00, LS08e, MFB04, MR02, MGLL03, RI07, RP02, XL02]. treatments
[CEP07, DWNB01]. tree [GY08]. treecode [DK01]. Trends [SRB06].

triangulation [BHH+09]. triazines [ZX04]. triazolinones [WZY04].

tribenzo [GLRL02]. trichloroacetaldehyde [CU01]. tricoordinated
[LTF+07]. trigonal [JHMB+09, JHMB+11]. trimer [LZJ03, RRCA08].

trimers [ABYM08, VS02]. trimethylamine [CPDZH08]. trimethylsilyl
[LLK06]. triose phosphate [AGK03]. tripeptide [VKP+08].

triphenyl phosphate [GS04]. triple [PP08a, RPNJ07]. triple-decker [RPNJ07].

triplet [CZ05, CG08, FDSA00, LS08a, OS06]. tripodal [HA04].
trisaccharide [GBB07]. tRNA [GGT08]. truncated [KK08a]. Truncation [RRS09, MN02]. Trypan [SRK+00]. Trypsin [JZD+09, CWV+05, MBC08]. Trypsin-ligand [JZD+09]. tryptophan [HLC09, Li01, LL01, MM05]. Tsi [XFF06]. TTTO [JW12, SLHW09]. tubular [FL07]. Tuczek [Ano06a]. tumor [WCF04]. tumor-specific [WCF04]. Tuning [JHMB+09, JHMB+11]. tunneling [Chu07, MKT04, 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, Sto05, Van02a, Van02b, YFR05, dSR08]. two-body [FGD06]. two-center [BRS07, GGA00]. two-component [Van02b]. two-dimensional [CVR08]. Two-electron [PFB05, Yas08, FR06, GYMN07, GGA00, Lai07]. two-electron/four-centers [GYMN07]. two-state [KT02, Sen06]. type [Bie04a, CXZ+09, CJK09, CVVB04, EdlVR+03, GC02, Gri06, HLC09, IKN08, KDG+09, Leh06, MY08a, OON01, SDL+09, TDG00, 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 [ZHMMW09]. ultra-incompressible [ZHMMW09]. 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, 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, HDMD05]. Unorthodox [KBB09]. unphysical [OV03]. UNRES [HXL09, NCO+05]. unrestricted [YH07]. unsaturated [BS03, KFD06, MTB09, Wan09, ZKZ+07]. Unusual [XK08]. UO [IV04, IVV06, RD+08]. Update [BKS02]. updated [Chu07]. Updates [An04b, BACJCT01, DV01, Gly06, JVK09]. upon [OFIK09]. uracil [LMGO+09, MSBS01, MHS05]. uracil-base [MHS05]. uranyl [IV04]. Urea [SK05, AS00, VVS07]. ureases [ESM06]. Use [BW1+02, DW08, Won00, ALB09, FC06, JNY08, KI01, MRC03, OCP02, PRK05, PRS04, RCL02a, RSN+02, Ru07, SH07, SVT09, VGGMM05, YTH01, YZ04]. used [DV00, ESP04, HDMD05, HD06, HD06]. user [DGD05, JKI08]. uses [KBB09]. Using [CSD04, FSO09, HL08, Kne05, LL07, M001, OSH03, QLHL09, SWR06, XSSC06, XLC08, XOW+00, Adc04, 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, GPS06, GGLR00, Haf08, HWDB03, Han01, HSMT04, HMSM06, HMMS09, HG08, HHP04, Ii02, IS07, IS03, IT03, IK00, JBGK08, JIK09, JVVK09, JTR05, JFG04, JSHG07, KRM+02, KKG+09, KM00, KLH+04, KK08c, Kle02, Kle03, KBT03, KKS04, Lab08, LCKL05, LCC09, LZ05a, LLL+08, LZCC09, LS05a, LZ05b, LSY02, LKW04, MWL+08, MT03, MMLC05, MKT04]. using [MV06, MBP09, MOP+07, MTE04, MRS09, MRS+07, NCO+05, NINAT+07, OFB08, OKE+02, PMB04, PS09a, PAT+09, PP08b, PDS01, PZS04, PSS+04, RI07, RI08, RMP01, RG08, RON02, SPG08, SSB+03, Sch00, SRC03, SBG+09a, SY09, SPT07, SMV+09, TP01a, Tie09, TCS03, UBDPJ04, VSW+03, Van02a, WLZ+07, WL00, WEE01, WG02, WOC+03, WCS09, XLT07, YK00, YYW07, ZCS04, ZBS03, ZWP08, ZHH09, vdVGDJ00, PRSMM02]. utility [KMH02]. utilization [GS08, DMLI05]. utilizing [NYTH09, Wan09].

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valinamide [HJCP01]. value [FPG+06, TBSM09]. values [OS06, PMPGP05]. vanadium [PV07, Tie09]. vapor [PHJ+08, UNM+01].

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[MR02, AB09, Chu07, GY06, HddMS05, Hds06, HD06, RS07a, RS07b]. Variations [TGGP+00]. variety [SBL05]. various [BP07, HMMS09, IT03, Kr06, KS01b, LML+08b, PP08a, PFJ+03, PMM05, RR05, WHH+06, ZCL09]. varying [CC09]. VASP [Haf08].

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vibration [CCL06, LSY02, ZWPR+04]. Vibrational [BP07, CLP+05, LC09, NR04, WB07, BRV+07, DB07, GBDP05, Gra07, Han01, HNR08, JARM02, LMB08, LN01, MR02, NRKH02, NAT07, PZWG+04, Tor02, WM04, WM01]. vibrations [CPDH08, DR09, KCL06, vE01]. vibronic [BP07, CLP+05, LC09, NR04, WB07, BRV+07, DB07, GBDP05, Gra07, Han01, HNR08, JARM02, LMB08, LN01, MR02, NRKH02, NAT07, PZWG+04, Tor02, WM04, WM01]. **vibronic** [TP01b]. view [CSJD04, Jac09, JMD+02, MGCA07]. VIII [EBD+01]. vinyl [YYW07]. vinylphosphine [MGLDS00]. viridis [IN01, OON01]. virtual [GFS05, KSM05, LZ05b, PRDS08, YOB+08]. virus [AJNG01, DLRZ09, KCL06]. viscosity [ZP03]. Visualization [MMP+07, RP07b, ARL01, KLY03, PGH+09]. Visually [SD09]. VMD [Pra01]. VMFCI [CCL06]. VO [PV07]. voltammetry [KJP+07]. Volume [Sta00, BVW04, LFSB03a, LFSB03b, Mue01, QNF09]. volumes [BHH+09, Rao00b, SBLK01]. Voronoi [GHBB04, MVLG06, SBLK01]. VP1 [KCL06]. VPP700 [KSY+00]. Vpu [KF08]. vs [CXZ+09, LLKC06, MA05, SCG04, Wi04].

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