Title word cross-reference

($\Phi, \Psi$) [WD04]. ($\varphi, \psi$) [TTB01b]. $-2$ [ZZZ+06]. $-4$ [ZZZ+06]. $1$ [FROD08]. $1/r^p$ [SG01]. $12$ [KGL07]. $139.00$ [Sta00]. $14$ [LMGR06, ZGXX06]. $16$ [HXD08]. $2$ [DMC05, GdAcV+07, LW04b, LXZ06, LW06, PF06, SFC04, WDZS07, YNW05, hYDN+08, ZTS09]. $2 \leq N \leq 372$ [Pul05]. $3$ [Lip00]. $3$ [BAH+02, FROD08, GDPCPU07, GdSuM+07, HP05, mJlZyL+08, KSN01, LYZ+08, MP03b, PF06, SHBD05, SFC04, TJM+03, WLL07a, WDZS07, XLL+02, ZLY07]. $3_{10}$ [JS07b]. $3d$ [Hol05, LD05a, Wu06, SZT08]. $4$ [FHF+01, LLXS02, QB05, WDX+02]. $4,7$ [ZWS+02]. $4d$ [ABY08]. $5$ [ZXL+04]. $5d$ [HZ09]. $6$ [Han01, LLXS02]. $7$ [LMO09]. $8$ [KSN05a]. $9$ [UM03]. $n$ [VKP+08]. ## [BRV+07]. + [FKS+09, GLRL02, GPSP06, GWL07, HDO+02, ITS06, KT08, LMO09, Mck07b, PV07, Sha02, WWT08, ZWY+09, ZL05, dRLMS00]. +2 [PNG08]. - [Bac09, Dib05, HTN03, LYZ+08, Mas01a]. 1
[AGI+07, IS03, LTD+02a, XZ04, ZX04, ZLLS04b]. 125 [HWFN01]. 13
[FH+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, FHR07, GPS06, HLB09, KRLD09, Kri08, ROG00, TFZRG01]. 2-
[IvSV06, JD09]. 2 [Gog08]. 3 [BPC01, LTD+02b]. 3+
[BTP09, BL00, Kri09b]. 5 [WC08]. 57 [HLLN06]. α [VBS09, CJW+09].•
[Mui05], ISQ [Bac09], 1/2TClP1 [BRDC02]. n [ZZZ+06]. p+ [GPS06]. 0
[DLF+02], 1
[BPC01, LDF+02, WLFP05, 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, DLF+02,
DRAS04, DRAS05, Dib05, DMM05, Don08, FJ08, GCCVB00, GBDP05,
GPS06, HYR06, HK07, Hua09b, IN08, IV04, IvSV06, IS03, JPF+00,
mJIZsLyL07, KZY09, KS05a, KKKJ08, KBL08, KS05c, LDMR01, LCO7,
LWK08, LLXS02, LW04a, LZZC09, LAT05, LF02, LTD+02b, LWY+09,
LM0909, MR02, Mas01a, Mas01b, MGLL03, McD08, Mck07b, MY08a,
NHY06, NHHN06, Owe05, PGNG03, PGRNG03, 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, WLS07, WLL+07b, WD08, XF06, YTY07, YLW+08,
YLW09, ZY01, ZL04, ZLLS04b, ZWL+05, ZLLS06a, ZLLS06b, ZKZ+07,
ZXY03, ZX09, doMSL01, dRLMS01]. 20
[Ber03, CCB04, Ell07, GB02, Var09, WLFP05, WL09b, ZZZ+06]. 6
[dOMSL01]. 2 [LMCD09]. 2+ [GHLK+02]. 2 [GYMN07]. 2 [YKK09]. 3
[BPC01, CPJ00, DRAS04, DMM05, FJ08, GBDP05, GD06, HLLS05, HYA02,
HDO+02, HTN03, ITS06, mJIZsLyL07, mJIZLy+08, KZY09, KT08, KKKJ08,
KSTC01, LDMR01, LD05a, LMK01, LDC+07, LW04a, LWW+06, LF02,
LWW+09, MR02, Mas01b, MGLL03, Mck07b, Mui05, NA06, ON07, PGNG03,
PGRNG03, RD00, SAS05, SLL+04a, SM06, SC08, TJM+03, TK08,
TDS07, UTM+02, UTT+04, VDM06, WDS06, WLL+07b, WD08+02,
XDS06a, XFF06, YLI08, YLW09, ZJM+07, ZZZ04, ZLLS06a, ZZW+07,
ZZW+08, ZZY09, ZZZ+09, ZKZ+07, ZWS+02, ZX08]. 3–n
[mJIZLy+08, KSN01, WLL07a, WDS07]. 36 [CS01]. 4
[DRAS04, DMN05, IN08, IvSV06, JD09, LDMR01, LMK01, Mck07a,
PHH+08, TY0505, TK08, UNM+01, UTM+02]. 4–n
[FH+01, WD+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,
RPJ07, SLL+04b, TY0505, XB08]. 6–n [Han01]. 60
[CJS+03, Ell07, KJ+07, Owe05]. 62 [HK07, STC+08]. 64 [CTFC08]. 4–
[CTFC08]. 7 [HYA02, LZZC09]. 8 [GZ07, Mck07a, Mck07b, PLC08, WLL01].
80 [KSN01]. 9 [Mck07a, Mck07b, PLC08]. 90 [NSO+07]. A
[Sa02, KKS04, MK02, ZPL07]. cam [ZAT07]. carbene [HA04]. h [WLFP05]. i
[OS08]. m [LYZ+08]. N [BP01, BS05, HTN03, MG00, Owe05, RC04, YT04,
DRAS05, FHF+01, Han01, HXD08, mJiZYl+08, KS05a, KSN01, LLXS02, LMGR06, LMO09, Mas01a, Mas01b, QB05, Tjm+03, UM03, WLL07a, WDZS07, WDX+02, XLL+02, ZY01, ZXL+04, ZXY03, ZGX06. s [WLL01].

β [AGO02, APG05, BTP09, BCP04, BSP06a, CSJ01, CJW09, CLA00, ESM06, GTC06, GAS04, HL08, IGNH03, KF03, LLW02, MCF07, MML+06, MS03, MK02, PP08a, PGC05, PSF+08, PMM05, RMP01, SBG09a, TFZRG01, Van08, WCF04, ZWPR04]. 3 [MH09].

Δ [CFR06]. ΔΔ [AGI+07]. η2 [KJP+07]. η6 [FKS+09, GM01]. f [ASS+02]. g [KRM+02]. γ [HL08, Iko04, TK08]. & [DLW06]. λ [CN03, KB09]. ↔ [UCT+03]. m = 1 [LYZ+08]. μ3 [KJP+07]. N [BY06, CCK01, GS09, HT05, HRBKB03, HJC01, JD09, KK09, KKH+07, KKO1a, MMPK01, ZPL07, MM07a, MM07b, VVBV02]. n = 0 [FHF+01, mJiZYl+08, KS01, LLXS02, Tjm+03, ZZX+06]. n = 1 [Han01, KSO5a, UM03, WLL07a, WDZS07, WDX+02, XLL+02, ZXL+04]. n = 1, 2 [DRAS05]. n = 14 [LMGR06]. n = 2 [QB05, ZGXX06]. n = 4 [HXD08]. n = 5 [LM09]. n = 8 [LMGR06]. n d(n+1) [GPSP06]. o [OSA06]. Φ [SO09]. π [Ang09, BY06, CXZ+09, DMZTO9, EFQD09, GYM07, HIM07, IINK09, LC09, LF07, MM05, OO08, RRCA08, SSS+09, ST01, WRP+06, Wou00, WJ00, YTH+07, ZGZX07]. π+ [Ang09, XZ04, ZX04]. pKα [KK08b, SMG09]. Ψ [SO09]. → [Ang09, CMD+04, Gog08, HTN03, LW04a, MGLL03, PGGN03, SOOF05, SLL+04b, ZL04]. s [ATM+07, GRO+03]. s/d [Hol05, S2T08]. σ [CXZ+09, HIM07]. sp2 [TTB01a]. V [Ang09]. x = 4 [KGL07].
[IGNH03]. -Helical [CPML08b, Van08, PCO+07b, PCO+07a]. -Helices
[IGNH03]. -helix [JS07b]. -hydrogen [ZGZX07]. -jul [KK01a]. -lactamase
[AGO+02, APG05, SDM02]. -lactamases [ESM06, MK02]. -lyase [PMM05]. -maltotriose [SWBM08]. -mercaptocarboxamides [TFZRG01]. -metal
[Wu06]. -methoxycarbonyl [KK09]. -methyl [CCK01]. -methylacetamide
[MMKP01]. -methylimidazole [HT05]. -methyloxaziridine [ZPL07]. -Mn
[AZM02]. -peptide [BSP06a, CSJ01, CLA+00, ZALMG03]. -peptides
[BCP04, LLW02]. -phthalocyanines [LS02]. -pleated [PGC05]. -porphyrazines [LS02]. -quartz [ZWPR+04]. -R [LZZC09]. -radical
[ZXZ+09, ZXZ+09]. -scaled [CN03]. -sheet [KF03, PP08a]. -Si [TK08].
-sigmatropic [LLKC06]. -SO [ZZW09]. -stacked [RCA08]. -stacking
[WRP+06]. -step [DLW06]. -strand [GAS04]. -substituents [PSF+08]. -TCNE
[GYM07]. -tensors [KRM+02]. -terminal [KK01a]. -the
[VHRR07b]. -TMPyP [AZM03]. -turns [HL08]. -type [OON01].

/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, YI04]. 1- [CUS00]. 1-aminom-3-propanal [FDSA00]. 1-jk
[SPCS08]. 1-naphthoic [CMLS05]. 1-pK [ZCS04]. 1-X-bicyclo [BPC01].
1.0 [AGSFA+05]. 10-endoperoxide [CG08]. 10-membered [ZW09]. 1174
[WWC+05]. 12 [HDO+02]. 12-crown-O [HDO+02]. 1291 [ANO06a]. 1328
[ANO05b]. 142 [ANO06b]. 1629 [WB04a]. 1Z [Lu09].

2 [BL08, LBG08, MM02, PFR04b, HÖF05, HTN03, MG00, P003, RC04, WC09].
2-allyl-2 [ZGZX07]. 2-aminom-2-imidazoline [XKG+05]. 2-amino-2-oxazoline
[XKG+05]. 2-amino-2-thiazoline [XKG+05]. 2'-aminoarabininucleosides [BL08]. 2-Aminopurine [SC01].
2'-aminoribonucleosides [BL08]. 2'-azido-2'-deoxyribonucleoside
[PFR04b]. 2-chloro-2' [JKM08]. 2'-deoxyguanosine [MM02].
2'-deoxyribosyl [LBG08]. 2-difluoroethane [CUS00]. 2-dihaloethanes
[WFR08]. 2-dihydro-pyrimidiny1 [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
[XKKL03]. 2-substituted [OSA06, WW04]. 2-thiouracil [LMGO+09]. 2.0
[GZM09]. 21C7 [GLRL02]. 21D8 [UTH+03]. 22 [Bo01, Qua01]. 24
[ANO06b]. 25 [Kne05, WB04a, WWC05]. 26 [ANO05b]. 27
[ANO06a, ANO06c]. 28 [HNWF12, Van08]. 2B6 [LCC09]. 2B6-substrate
[LCC09]. 2H [dSVA+09]. 2H-tetrazole [dSVA+09].

3 [AAP00, KAK+09, LEV+09, NYTH09, Rud05c]. 3-butadiene
[Hir08, WR07]. 3-dihydroxypyridine [YXZ+04]. 3-dimethylallene
[ZPL07]. 3-fluorobutanal [NSB08]. 3-hydroxy-2-mercaptopyridine
[YXZ+04]. 3-trimethylsilyl-1-pyrazoline [LLKC06]. 311 [Wib04]. 31G
[BRV+07]. 31G* [RRP+01, FKJ+01, NL08]. 31G** [WD04].
31G*/AMBER [FSFK05]. 34 [PHH+08]. 3a [HKHN08]. 31G*
[RRP+01, FKJ+01, NL08]. 31G** [WD04].
31G*/AMBER [FSFK05]. 34 [PHH+08]. 3a [HKHN08]. 31G*
[RRP+01, FKJ+01, NL08]. 31G** [WD04].

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].

5 [LDY+08, PFR04b, PMM05, TAS07].
5-di-tert-butyl-o-diiminobenzosemiquinonate [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].

6 [BRV+07, Wib04]. 6-311 [Wib04]. 6-31G [BRV+07]. 6-31G*
[FSFK05, RRP+01, FKJ+01, NL08]. 6-31G** [WD04]. 6-bisphosphatase

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

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

9-heterofluorenes [CZFH07].

= [Bac09, CPJ00, CRC+08, GHLK+02, GPSP06, Han01, HT05, HYA02,
HKHN08, HZ09, Hu09a, JJK+00, KBL08, LS08a, LZZC09, LYH+08, Mar03,
Mck07a, Mck07b, OS08, RB01, STC+08, WLLS04, WZZ+09, WD08, WWS07,
XFF06, ZJM+07, ZY01, ZXY03, ZL09b].

A*0201 [WCF04]. AA [KB02, KDSV02, POJ01, PB05, XLT07]. AA/L
[KOML08]. Ab-initio [Haf08, HELM09]. abasic [FPN+05]. ABEEM
[YZ06]. ABEEM/MM [YZ06]. abilities [OYH09]. Ability
[GM01, RRZA08]. ablation [KZW+05]. ablation-mass [KZW+05]. ABO
[WD08]. **ABSINTH** [VP09]. Absolute

[BWE05, ZM09, BMRF01, DHF+05]. absorption

[MWL+08, MSH+06a, YXZ+04]. abstraction [AST06, CUS00, CUSS03, GAIM+01, mJlZsLyL07, LW04a, LLL07, TGLL07, WLLS04, XLL+02]. Ac [GHLK+02]. accelerate [Gon07]. Accelerated

[LSG06, LDG02, FSM09, Hass04]. Accelerating [FEV+09, LEV+09, SPF+07]. Acceleration [KG02]. accelerator [ATMK03]. acceptance [KBB09]. acceptor [BL06, RM07]. accessibility [AG03, ENM+04, GP06, Tots04]. accessible [BHW00, BMLV04, GB04, HHS+05, LFBSK07, RP07d, TSMNG01, TRS02, ZCL09]. accessible-surface-area [ZCL09]. Accompanying [Ish02]. account [May07, SN06, Vya01]. Accuracy [FII+07, GG09, PSMB05, SKK+07, UBPDJ04, Bie04b, FKFG08, JS07b, KC01b, MKGA06, MHW04, RK05, SM03, SW06]. Accurate [ABWT09, BDPRMAI00, EK06, Gk09, Gri04, HD06, HMM06, Ish04, LLZL09, MSH+06a, Tots04, WFHP01, WHP02, WHF08, WX09, ALKH04, Bie04a, BLB09, CBGB05, CF06, GKK07, Hdd05S05, JKK+00, Rud05a, Rud05b, Rud05c, Vas02, WC08, ZFW08, vEMK01]. accurately [IGL07, SBI08]. acetaldehyde [Lu09, YLZ08, Lu09]. Acetalization [RUPH06]. acetics [MG06]. acetamide [CCK01]. acetate [GWM08, PGG06]. acetic [MH08a, YT03]. acetonitrile [ELK+09, GJK00, NL07]. acetylcholine [GCD+08, MCH05]. acetylcholinesterase [MCK05]. acetylcholinesterase-catalyzed [MCK05]. acetylene [DL+02]. AcF [GHLK+02]. acid [CJ+02, CML+05, CJK09, CCK01, DP03, DP04, DLHC06, DW+07, FZL07, HFHL06, HLC09, IT03, IKYM09, JPF+00, JKM08, JCL05, KLB03, LL07, MT03, MMLC05, MSF+08, MHO0a, NAK07, NHH05, NLL+09, Pac06, RR05, RKK03, SKGS00, SYC03, SL04, SWB09b, SWR06, SHK+05, UNHYT06, VM02, XSHC06, XLC08, XLT07, YTO3, YXL+09, ZYZ07, ZHZ08, ZOJ+06, vDSSvA04]. acid-3 [vDSSvA04]. acid-catalyzed [RR05]. acid-nucleotide [MSF+08]. acidity [ELK+09]. acids [BE06, CADW03, CLA+00, FM00, HWT03, HP04, IKYM09, KSO1a, LDV+08, MB00, MM05, NHH05, OMNH08, PPG06, VAN02a, XKK00, YLL+09, ZLD09]. AcO [GHLK+02]. across [HZX04, SSM08, SRB06]. act [GM01]. actinide [AB00, GHLK+02, NS0+07, VMA03]. Activation [EL06, BGC+09, BLZ05, CC09, CFER04, KTO8, Lu09, PV07, RRS06, Vya01]. active [AG00, BSDM04, CFR06, CF+09, FCP+04a, FCP+05, HBM06, HFS+07, HYR06, JHPRSM+05, KSK00, KZRO03, LLL03, MDA08, PSM06, RZWS07, SSO5, SFR07, TDD06, XLL08]. active-site [SFR07]. activities [HMM09, MS04, ZWB09]. activity [AGMPRG+08, Bou01, CW02, DD08, DA01, DW+08, DW+09, FTLV01, GDP08, LC09, MRS09, Sha02, WZY04, Zor08]. acylation [MCK05, MK02]. adaptable [KF08]. Adaptation [HLM05]. adapted [FCP+04b, HDS06, HD06, LWX07, PTC01]. Adaptive

[BHW00, HBW00, HBW01, HW03, HLSH05, DK01, GY08, OM04, RNG03,
addition
[BL06, DG07, LL00, Mu05, RALL09, RR05, WC08, WSC09].
addition-elimination [Mu05]. additions [AVB00]. Additive
[GGK08, CCK01, LKA01]. adenine [KKMMS04, SG07a].
adenine-thymine [KKMMS04]. adenosine [MR07, YK09]. ADF
[tVBB01]. adiabatic [SLRC01, TVL03]. ADMA [EM03b]. admissible
[WG02]. adrenergic [YK09]. adsorbate [BWI02]. adsorbed
[DR09, PB00, XPW09]. Adsorption [ATH03, BR00, BS01, HS08,
ZTP08, NK06, SUR06, ST04, WLX05, ZCS04, ZS05]. Adun [JGVF05].
advanced [MM07, YK09]. advances [MM07]. Advancing
[PP8b]. aect [AST06]. anities [AVS09, DJ04, KS05a, KKMMS04,
LLXS02, MR07, YK09]. anity [ABA04, FO08, GCD08, KFB05,
KS08, Lee09, LX09, MMR06, RTG00, SOF05, SWV05, ZWS09].
affording [OY01]. after [TJ03]. Ag
[GPSP06, LYZ08, NA06, SG07a, WC08]. against [SSS09]. AGBNP
[GL04a]. AgBr [Sha02]. agent [LH06]. agent-based [LH06]. aggregate
[KHF09]. aggregates [AB08]. aggregation [IM06, OGH05].
AgN [ZX08]. agonists [GCD08, SBG09]. Agreement [LS05b]. aided
[PJ07]. AIM [SFC04, CFS03, WW03]. AIM2000 [An01a, BK502].
AIM2000-Program [BK502]. Al
[OS08, WZZ09, Van08, KKH08, QB05, WZZ09]. al. [RKH03]. Ala
[PC00]. alanine
[DSR07, ECA06, GAIMV01, GS09, GKT04, HHP04, HMK02, JW06,
LSW01, MOP07, MFR07, PFJ03, Qua07, WD04, ZW09, ZM06].
albicans [RGP07]. Alchemical [Blo04]. alcohol
[FBDG06, JH01, KBN02]. alcohol/water [FBDG06]. Alcohols
[ACLD03, LCA03, LCGA03, LCA03]. aldehydes [GLA01d]. Alder [HR08].
algebra [AT02]. algebraic [Tor02]. Algorithm
[GG307a, GGB07, KS03, MO11, WM12, ASGW07, AM06, AM06b,
AGSFAL05, BP02, BED02, BA08, BMTC01, BSH07, BHH09, CS02,
CLX09, CWV05, CF04, DDKV07, DP03, DP04, DSR07, DVB07,
DAA08, FKFG08, FCP04b, GF08, GLD08, GCD04, GM04, Gon07, GKK07,
HH03, HH04, HM06, HLM05, Ish04, IPN06, IPN07, JCA02, KH01,
KM00, KMA07, KUB07, KvGH01, KH06, LJZ07, LJS05, LM03, LMO09,
MP03a, MP03b, MVL06, MM07, Nak02, OR05, R06, RPH09, SKSH07,
SJY04, SW06, SSM09, Ste04, SBH02, T002, TGD05, VGO07,
WVB03, WSC09, YK00, YGZ05, ZBS03, Z08, ZA07, vLB02].
Algorithms [LM09, BYQ03, BPRM00, CKMC04, CSRST04,
CHM05, DB06, FS98, FS00a, HWDB03, KOFF09, OLT08, OGH05,
RL04a, SE08, TP01a, VW04, WK01, YL06, vLB02, HB00, HB01].
alignment [BA08, CLZ09, CLX09, HHG09, R07, VGDU08, Leli06].
alignment-free [VDU08]. aliphatic [MS04, SDV01]. alkali
[JHM09, JHMB11, WWT08, ZWY09]. alkalimetal [BS07]. alkaline
[JHM09, JHMB11]. alkaloid [BMR01]. alkane [HMB04]. alkanes
alkyl [BE06, CC07, EB04, LLZL09]. alkyl-cyanobiphenyl [CC07]. alkylation [EL06, VBGL+00]. alkynes [WCW08]. All-atom [FM00, MB00, VGO+07, GB04, IT03, MT03, PHH+08, RG08, WS07, JS07a].

All-electron [EL09, IN+05, IS07]. all-purpose [JG07, SF+05, AB+07]. AlNC [MLCD01]. alpha [GKK07]. Alpha7 [GCD+08]. AlPO [PHH+08]. altered [DLRZ09]. alternating [YFR05]. alternation [JPCA08]. alumina [LST08, LTV08]. ammonia [HT05]. ammonolysis [UNM+01]. among [IGNH03, LLL07, WS07]. amorphous [CA04, CA07a, CA07b, SH07].

AMP [FKM+06, FKM+07]. amplitude [KS05a]. Amyloid [BTP09, MS03]. amyloidogenic [CP09]. amylase [NK01]. anabolic [AGMPR+08]. analgesic [CMBC08]. analogs [AS09, BCE05, FPG+06, FKJ+01]. analog [LRI+02, WC08]. analogues [BSB02, WHP02, XY+06, ZSE08]. analyses [BLT03, CZ05, DRAS05, HN02, HR08, RP09]. Analysis [CGsdST06, EKO+01, HG08, KS01a, LWK08, UTM+02, UTT+04, hYDN+08, AJNG01, ALB09, AVS09, BM07, BLF02, BL00, BAH+02, BPCD07, CG03, CS01, CCM+04, CSRST04, CA07b, DKV07, DRAS04, DS+07, ECM+03, FK07a, FC06, FSS00, Gly06, GS07, Gra07, GHB04, HHWG08, HS00, HSLH05, HP05, IN08, JMF+00, JMD+02, JFG04, KB02, KK08a, KMH02, KS03, KN04, KSK00, KMA+07, Kn00, LRF+02, LSO5a, MGCA07, MS03, MWE02, MHW04, MPP+07, MA05, NK06, NSU+02, OML+00, ON07, PFC03, PGH+04, PP08b, PYEA03, PAS07, PYCD03, PYS05, PC07, PLC08, RMHK03, RS07b, SH09, SMGE08, SSH03, SFC04, SCF+09, SvdS01, TYN05, TCR+02, TT01, TD06, TTB01a, TTB01b, UTH+03, VGB08, VKCK09, WRBV03, YNW05, YK08, ZSE08, Zer08, ZWB09, ZHH09, ZB07, NYK+09, Ruv07, VB09, RS07a, VB07]. analytic
Analytical [HNWF97, HNWF12, PDC+08, QCK01, QCK02, RLR+04, WL02, DSR+07, HC08, HHS+05]. analyze [AGMPRG+08, Ham07, MCF07]. analyzing [DW08, LD05b], anradite [ZWTP+08], anesthetics
[ASGW07, DOSG06, GL04a, IK00, KBT03, LFSB03a, LFSB03b, SJW09].

ant [CLZ+09, CLZX09, DKV07]. 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]. antigenic [WCF04]. antiinflammatory [CMBC08]. antilipid [MRS09], antimicrobials [GDPP08], antitumor [KC01a, WM01].
XWC09, XKKL03, YS00, YK08, ZS04, ZS04. Approached
[LL07, XSHC06]. approaches [BP07, Con02, CSD05, COL+06, MLJ03, PSF+08, PMM05, RLD09, RSS09, SM08a, YCW+09]. appropriate [Bac07].
approximate [Cu08, GB04, Hol05, KS02a, SZT08, SYC03]. approximated [PSF+08]. Approximately [EA06]. approximating [MR04].
approximation [AB09, BRS00, BRS01, CLP+05, CCK01, Der09, EA08, GMA04, GWS+02, ION07, Kri09a, Lai07, LFSB03a, LFSB03b, LN01, MTE04, Nee03, OCB02, RR07d, SHSF05, ZFL+05]. approximations [Dya02]. APS [CBC+08]. APX [ZJM+07]. aqua [RMP01]. aqua- [RMP01]. aqueous [BISB02, CPJ00, CPJ01, CW02, CCK01, DA01, EK06, FHRR07, HMWC03, HRR05, HDO+02, IV04, IvSV06, JM07b, KEH+02, KPR04, Kri08, Kri09b, LRI+02, LR03b, Loe03, LMIF06, MM02, NL07, PK04, PHRR08, SH09, SMK00, SBB02, VP09]. arabinonate [RGP+07].
arabinonohydroxamate [RGP+07]. arbitrary [KH06, LMV07]. architecture [TDK07]. architectures [TYO+02]. area [GCD+08, GB04, HHS+05, Lab08, LFBSK07, RP07d, VP02, ZCL09]. areas [BHH+09, TRS02]. arene [FKS+04, PCMG09, RRZA08]. arene-containing [RRZA08]. arginine [CJPZ08, SMGE08]. arginine-bound [CJPZ08]. argon [BWW+08]. argument [Ish04]. ARIs [PS09a]. arising [CCSJ00]. armed [KLM+09]. ArOCS [ZGXX06]. Aromatic [CPML08b, PCO+07b, Van08, Bor03, FVB08, HLC09, MM05, MGMM07a, ST01, SMV+09, TDK07, VS08, WFHP01, XLT07, PCO+07a].
aromatic-type [HLC09]. Aromaticity [BPCD07, FMP08, 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, DINAT+07, TCSM03]. arylamide [VIP+06]. ascorbate [HBM06]. ASIC [NYTH09]. aspartic [ZZY08]. Aspects [HBB00, M001, BMRRD01, BRS07, SIE01, TT02]. assemblies [DFGB09]. assembly [DPRR05]. Assessing [IB04, FGR07]. Assessment [BP03, CCWH02, DGI+08, KS08, LWH06, SSS+09, WSM+08, CKMC04, FMP08, GT03, LLS03, SP05, GGT08, GHB04, TFZR01]. assignment [BB05, BMRF01, PR02]. assignments [PF06]. assisted [BA04b, KT08, WXJ+05]. assists [BM07]. associated [SWR06, TT08].
Assiative [ABYM08, NL08]. asymmetric [WR07, WFR08]. Asynchronous [GLP08]. atmospheric [GCCVB00, PGN03]. Atom [RPO7a, RM00, BPC01, BR04, BWW+08, CCK01, FM00, GWS+02, GB04, HLLS05, IT03, J07a, mJZyL+08, LMK01, MT03, MB00, PHH+08, RG08, RS08, SSB+03, SBLK01, SLL+04a, TGLL07, VK06, VGO+07, WLL07a, WBSR03, WS07, WLL+03, YLWL09]. atom-bound [VK06]. atom-centered [SB+03]. Atomic [DVP+02, FDM00, AS00, Bac07, BSC+01, BCNS07, BS06b, BK00, BLT03, BAA07, CN03, FS04, GC02, Ish03, JBB00, JJB02, KRM+02, Kau07, KS01a, KC01b, Lab08, LMV07, LST08, LTV08, N09,
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, mJzsLyL07, KGN07, KS02b, LDC+07, Mat03, NSO+07, RP07b, RRP+01, RLR+04, RLER04b, SO09, SNM+06, SFC04, Wil01b, WDX+02, XLL+02, PFB05].

Atoms [VM07, YK08, ALTB06, AD00, ASS+02, BHTCG07, BKS02, BS03, CMJ08, CDS09, EdlVR+03, FS04, HSF08, mJzsLyL07, KGN07, KS02b, LDC+07, Mat03, NSO+07, RP07b, RRP+01, RLR+04, RLER04b, SO09, SNM+06, SFC04, Wil01b, WDX+02, XLL+02, PFB05].

Atoms-in-molecules [VM07, YK08, RLR+04].

ATP [FCP+04a, GS04].

ATP-binding [GS04].

ATP-dependent [FCP+04a].

ATPase [HLB09].

attachment [LBG08, XWXC08].

attack [CBS+03].

Attaining [Rud05a, Rud05b, Rud05c].

attending [HT05].

aug [Wib04].

aug-cc-pVDZ [Wib04].

Auger [OKE+02].

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

autoantigen [KVS+06].

AutoDock4 [MHL+09].

AutoDockTools4 [MHL+09].

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

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

automaton [XWC09].

auxiliary [GKH05, JSHG07].

available [SCF+09].

average [TRS02].

averaged [CP08, PYCD03, PYS05, PC07, PLC08, SMAdV00].

averages [Rap06].

averaging [BS+C+01].

avian [DLRZ09].

avoidance [WCFH02].

axial [OMNH08].

azaglycine [LKJ+04].

azide [MSR04].

azides [ZX08].

azido [PFR04b].

azole [SM+08].

azole-bridged [SMM+08].

azurin [PMGL03].

B [OS08, Sta00, WZZ+09, WD08, ZZZ+06, ALKH04, BAL+01, FH01, GL04b, JS07a, KVS+06, LMO06, Maz01, Pin03, VDM06, ZWB09].

B-DNA [Maz01, Pin03].

B-domain [JS07a].

B-spline [ALKH04].

B-splines [GL04b].

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

B3LYP/6 [FSFK05, NL08].

B3LYP/6-31G* [NL08].

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

Ba [WD08, XB08].

Bacitracin [Dra00].

back [BB05].

Backbone [CPML08b, GKK07, Van08, Adc04, Ano06c, AHGK09, CIWL09, HSWN01, KLS02, LKA01, MFB04, MLL08a, PCO+07b, SP05, WZW+06, YL06, PCO+07a].

backward [KM07].

bacterial [Ano06b, CPM03, Gs04].

bacteriochlorophylls [LKT04].

bacteriofephelopytin [N01].

Bacteriorhodopsin [RG02].

Bacterioidei [SDS02].

Bader [GHBB04, SKH07].

Baker [WB05].

balance [Ano06c, WZW+06].

balanced [BP05].

Balancing [CF06].

band [AJ03, JCA+02, ZZW09].

Baoshan [JW12].

bare [KT08].

barrier [CRGN07, KSTC01, LSG06, MG06].

barriers [DBM03, EL06, HFHL06, PBF09].

bars [MD+04].

base [CCK01, DP04, FZL07, HWTL03, KKMM04, MML05, MSF+08, MHS05, NL08, OY01, PG04, PSS+04, PSMB05, SKGS00, SMG7a, SBL05, SC01, SYC03].

base-catalyzed [OY01].

base-pairing [DP04].

based [Adc04, ALTB06, ALB09, BA09, BDPRM100, BMRF01, BDW00, BMTSC01, CGMPT+08, CKR08, CLZ+09, CLZX09, CFK08, CHA+07, CPU09, DUG09].

PPG06, PSMB05, RKA+09, SD01, TBSM09, UBDPJ04, VZVG06, VC04, XLT07, YOB+08, dGGC00, DVP+03].

atomic-centered [TBSM09].
bicyclic [EBDPM00]. bicyclo [BE07, BPC01]. bifurcation [CPL02]. bilayer [CEP07, HNL08, MCR08]. bilayers [JM07b, RG08]. bimetallic [WCS09]. bimolecular [ML00]. binary [Kle02, Kle03, LCSZ09].

Binding
[ABÄ04, AGO+02, BCP03, RGP+07, ABYM08, AM06b, APG05, AVS09, BWE05, BSP06b, DLRZ09, Dra00, ECM+03, FKS05, GCD+08, GS04, HT05, HNW07, HNW12, IO08, JMD+02, JZD+09, KFB05, KS08, LXW+09, MK02, MHS06, MLL+08b, MRS+07, NyHN06, NHN06, OHY09, OFIK09, PMGL03, RSP03, RG08, RK05, Ru07, SO0F05, STSF02, SVW+05, TGGP00, VGGMM05, WM04, WHF08, Won00, XL02, ZGFL01, ZWB09, KEB04].

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

bioinorganic [MSH+06b, SGD06]. bioisosterism [DPM09]. biological [CCK01, CMGDAC+07, GdAcV+07, HMMS09, LDTS07, Mac04, TH02, WCK00, YPNE09, vdVGDM00]. 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, LS004, OVMV04, WB04a, WB04b, WB05, WL09a, ZFW08].

biomolecule [ABWT09]. biomolecules [ECM+03, Est07, FEVM01, HMD06, KY00, MMLC05, QSS01, YNZ+08, YJF06].

biomembrane [WE01]. biomimetic [FO08].

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 [SSB+03].

blood [CRG07, HSM06]. Blue [CPDZH08, HRG07, CR02, MC08, SRK+00]. blue-shifted [MC08].

Blue-shifting [HRG07]. BLYP [TCT03]. board [ATMK03, KAK+09]. boat [R09]. bodies [FS98, FS00a].

body [CCK01, FII+07, FBGD06, Ike04, Loe03, SM03, TKH07, LR03b]. Bofill [Qua01]. Boltzmann [WB04a, WB05, ABWT09, BHW00, BHF09, BH03, BF04, BP07, GPN01, GCD+08, GGT08, H050, HB00, HBW01, KWHH07, LDG02, NYTH09, PZ04, SAT004, ZSM+08, WB04b].

Bond [CGMPT+08, CRC+08, JG03, MGCA07, May07, SH08, WM12, Bie09, BL06, CML05, CPLL02, CPDH08, CJW+09, Cus08, DR09, DG+05, DMZT08, FH01, FO08, GYN07, GR07, GS07, HRG07, HS07a, Hr08, JPCA08, JP09, Kle03, KBL09, LC07, LZZC09, LS08c, LS08b, MG00, OO04, Pac06, PSC+01, PAS07, PYS05, PV07, Ra000a, RM07, RC02a, RD00, SEK09, Sha07, Sim07, SPT+03, SWZ04, SMZW05, SSMW09, ST01, SSW+07, TJM+03, Tru07, VK06, VBGL07, WHR08, WJ00, WX08, vLBBR12].

Bond-based [CGMPT+08]. bond-order [LS08c]. bonded [CPDZH08, Gon07, HT03, IO08, LB05, LDL+09, LZF+09, MC08, 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
[CJPZS08, WC09]. Boundary
[BH03, ABWT09, Ara04, BVW04, BF04, BF07, HH04, KWHH07, QSS01, TK08, WM06]. bovine
[MBC08]. bowls
[MBP09]. box
[LM03, WM06]. box-counting-based
[LM03]. boxes
[BMP09]. 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, HSM06]. BrCl
[WLLS05]. breakage
[SWR06]. breaking
[HRR05, Pac06, VHRR07b]. breast
[VGDSU08]. Breit
[Sh03]. bridge
[CFC+08, PAS07]. bridged
[LHP01, SMM+08]. bridges
[KF03]. broadly
[PB05]. broken
[ATH+03, BB08]. bromine
[WyLG+09]. bromine-substituted
[WyLG+09]. BSSE
[GA06, PSC+01, SP01, SAM06]. BSSE-corrected
[PSC+01]. BSSE-free
[SAM06]. Buckminsterfullerene
[NRH02]. buckycatcher
[Won09]. Buff
[KS06]. build
[BMTSC01]. build-up
[BMTSC01]. Building
[BCIB05, BAA07, GKK07, HP05, MABM09, PC00, PFC03, Fau01]. built
[GSF05]. bulk
[BACJCT01, BGC+09, EBL+08, JBGK08, LZZC09, LLL03, PB05]. bulk-doping
[JBGK08]. butadiene
[GRO+03, His08, WR07]. butanal
[NSB08]. butanes
[WW04]. butyl
[Bac09]. C
[An00, BAL+01, BCP01, BSB05, Bac09, CTFC08, HK07, mJZyL+08, KYYW07, KJP+07, KSN01, LYZ+08, Mck07a, Mck07b, Owe05, SLL+04b, VBS09, WLL01, WDXS06, WZZ+09, XFF06, YHD+06, ATBS04, Ber03, CPDZH08, CCB04, CS01, CRSB03, CTFC08, DGD+05, DRAS04, Eil07, FFH+01, GYCZ04, GZ07, GB02, HBM06, HYA02, HK07, HA04, IN08, LDMR01, LMK01, Mit01, O004, PRSM03, PV07, RD00, RFSS06, SLL+04b, STC+08, TNY05, WLPF05, WDWS06, Wil01b, XDS06a, XWXC08, ZZL04, ZW09, ZLD09, ZZvRSC08, dRLS00]. C-PCM
[CRSB03]. C12A
[BRDC02]. C12A-p8
[BRDC02]. C96
[ONHN00]. Ca
[WZZ+09, WD08, XWC09, HL809, PNG08]. cabonyl
[RUPH06]. CaCO
[SCP08]. cage
[CS01, KFD06, WLPF05, WL09b]. cages
[CJS+03, Wan09].
calcium [HSMT04, HLB09, LGB+09, MHJS06]. calcium-induced [LGB+09]. calculate [BACJCT01, CSD04, IS07, Kar01, Kne05, KBLP09, OV03, RSN+02, SFRS01, WW03, YS00]. calculated [BE06, BE07, GG09, Gra07, LMV07, RSKSB03, RM00, Wib04, WM04, ZXY08, KI03]. calculates [ATMK03]. Calculating [Chu07, CG05, DRMD03, DF04, LN01, MC06, PDC+08, PMS05, RSE07, SYC03, WCK00]. Calculation [BK00, CPML08a, DJ04, KKY01, KRM+02, LSW+01, NT03, MO01, MRS+07, TS05, VM02, VC04, WKYY01, ZWP+04, BP02, BS+01, BH03, ECA06, FOL+04, FROD08, GKR+08, GLMV09, GAdGM08, GGT08, HTKG08, IL02, ITN+05, JJK+00, KFNH08, LFK05, MGLO03, NRRK+02, Ni09, OCP+02, PZW+04, PRSM08, RNC03, Rap06, RLER+04a, RKA+09, RRFC+03, SOOF05, SKGS00, STSF02, SM08, SHH07, TZX01b, TZX01a, TLOG00, TRS02, TKN+08, UK04, UIH09, WLL05, WLL+07b, WSM+08, WM01, XOW+00, ZWB09, ZL09b]. Calculations [YH07, Ano01b, ALKH04, Bac09, BP07, BS0B05, BMRDB01, Blo04, BMB07, BMRF01, BW1+02, CLP09, CMJ08, CN03, CRS05, Chi03, CS03, CMA+08, DB07, DPDG05, DSS03, DMJ05, DWC+03, EKO+01, EBL+08, EL09, FKG08, FLO8, FMSA06, FR06, FO04, GJL+08, GBDP05, GM04, GW+00, GB07, GPS06, HHHB00, HLLN06, HYA02, HMSM06, HFFL06, HKHN08, HT03, HWGB01, HZ09, Hua09a, Hua09b, IL09, IGL07, IP06, IPN07, JCA+02, JCGK08, JCS07, KGL07, KWH07, KRLD09, KT03, KBLP09, KS02b, KSK04, LLA01a, LLA01b, LL01c, LLA01d, LLA03, LFSB03b, LDC+07, LHI09, LW06, LC06, LKW04, LZF+09, LS05b, LG02, LM09, MLMC05, Mza08, MBL+00, MA05, MLCD01, ML03, MS01, Mui05, NYK+09, NTH09, NSU+02, OBB05, OYH05, OS06, OHR02, Oos09, OKE+02, PB06, PMGL03, PVDB00, PV03]. calculations [PBZ00, PRSM02, PSS+04, PSMB05, RSP03, RMP01, RP02, RRCA08, ROG00, RWBH09, RS05, RRS07, RJLR06, SB108, SSB+03, SCS07, SBC+09a, SHM04, Sha02, SSL02, SN06, SFRS01, SM09, SG01, TK08, TY03, UK01, UTM+02, VPK+08, VZVG06, Van02b, VE09, VIP+06, WL02, WTK06, Wo08, WC04, WIF08, WR07, WFR08, WH+07, WJ00, XLZ08, YTH01, YK08, YSA+03, ZSE08, ZXYF09, ZM03, vGGB00, vdVGDM00, LFSB03a]. Calibration [OKH+02, LLZL09]. calix [RRZA08]. camphor [AST06]. Can [DSB+02, DDBP09, LC07, MSH+06b, PB06, SBI08, STSF02, WS07, IG07, Mck07a, WC04]. cancer [VGD008]. Candida [RGP+07]. candidate [SF07]. canonical [BP07, EMP07, ITN+05, IS07, KM00, Kn00]. CAOs [PS03]. capabilities [GCD04]. capped [CZ05]. caps [ZC03]. capsid [KCL06]. captopril [AGO+02, APG05]. capture [YXC+07]. Car [JP09, Sch04]. carbapenem [BB00]. carbazole [YFR05]. carbenes [HA04]. Carbohydrate [KBB02]. carbohydrates [ACLD03, HR08, KD502, LR03a, LCD03, LCGA03, LCA03, LH05, MW00, Sto05, KYT+08]. Carbon [KK08c, LMGR05, BS05, BG07, CZ05, CDPL09, DWS+09, GKK07, HT05, KT08, KLS02, KK01b, LMK01, MMVH07, PAS07, wQZsLyZ02, SRS07.
carbon-centered [WSC09], carbon-rich [CZ05], carbonate [vDSSvA04], Carboxyl [RD00, DL00, LLA01a, LLA01b, LLA01c, LLA01d, LLA03], carboxyls [BRV+07, LMG05, PLC08], carboquat [WM01], carboranes [JR01, OSA06], carboxybenzoxazole [UTH+03], carboxylates [CJPZS08], CarC [BBSS06], carcinogenic [EL06], carcinogenicity [VS08], Carlo [AGSFAL05, AGSFA05, BR03, BHG03, Der00, FCK08, GHH07, HMD06, IM06, IKYM09, KKC05, LML00, LZA02, LL09, Nak02, NA06, NCO05, OM04, SKGS00, SCS07, SBJ08, SM08b, SWRW06, TS05, XKG05, ZCS04], Carlo-with-Minimization [NCO05], carma [Gly06], carrying [Tor02], Cartesian [LPK07, PHR05], CAS [PRSMM03, BMB07, JHPRSM05, PRSM02], CAS-SCF [JHPRSM05], CAS-SDCI [BMB07, PRSM02], case [AB00, AS00, BUMCMRL00, BWW08, CFS08, CJPZS08, MV06, MDI04, Pac06, PGG06, PC00, Pog03, RUPH06, SBI08, SN06, Van02a, WRBV03], cases [BCF09], CASPT [PO03], CASPT2 [KRLD09, WLZ07], CASSCF [Bac04, Bac07, DOSG06, WLZ07, dSVA09], CASSCF/CASPT2 [WLZ07], Catalysis [UTH+03, DWS+09, QZZZ03, TH02, VBGL00, WZ05], catalyst [VBGL00], catalysts [YX+07], catalytic [CGB+09, KSK00, LS08b, MS04, NT00, RWBH09, SPT03, WC08, ZAT07], catalyzed [AST06, BTP09, GVA03, GLH+08, HSWW00, MCK05, OY01, PHKG07, RR05, RH01, TGLL07, WCW08, WCHW09, ZWS09], catastrophe [PA05], cathepsin [ZWB09], cation [DSB+02, Don08, LB08, OO04, PV07, QZL+04, SLRC01, VL00, WLZ07, WSM+08, Wou00, ZL05], cation-water [DSB+02], Caticonic [JR01, TBG00], cations [AC08, GB09, GS04, GWL07, HIA03, HD05, NSB08, RRS06, SZT08, WTT08, ZYW09], caused [LPK07, TT08], cavities [BCIB05, BHH+09, IME02], cavity [RZRA08, ZFL05], C [CJW09], CB [FHF01], CBS [L09], cc [Wib04, GYM07], cc-pVTZ [WD04], CCH [ZKZ07, ZKZ07], CCl [ZLLS06a, FHF01, WDS07], cclib [OTL08], CCN [JDS06], CCSD [BBI09, Lu09, PFJ03, PV03], Cd [GPSP06, XB08, BMRF01, BB09], CD88 [UNHYT06], CDOCKER [WRBV03], Ce [SNM06], Ceccarelli [An06b], cell [Gou07, KVS+06, KS05c, LEV09], cell-based [Gou07], cells [CCC09], cellular [XWC09], CeN [VP08], centauric [PA05], center [BR05, GA00, IN01, La07, GMM07a, GMM07b, NR04, ON01, SGPS09, TBM00], centered [CC01, SSB+03, BSM09, WSC09], centers [GYM07, JKL08], central [CGM07, CM09], CeO [CCJ09], ceramic [HZA04], cesium [HD06], CF [mJZsLyL07, YLW09, LDC+07, gThDJ+01, UTM+02, UTT+04, WLL+07b, YLW08, YLW09], CFCI [mJZsLyL07], CF91 [TTB01a], CFMC [NCO05], CH [CP00, GB05, HT03, IN08, mJZsLyL08, LW04a, LDT+02b, MGL03].
Mui05, RD00, SLL+04a, TJM+03, WLL07a, WLL+07b, WDX+02, YLW+08, ZL04, ZZW+07, ZZL+08, ZZL+09, HKHN08, FHF+01, GD06, HLLS05, mJZsLyL07, mJZsLyL+08, KZY09, KKJH08, LW04a, LWY+09, MM05, Mas01b, OO04, OO08, SEKs09, SLL+04a, SSS+09, TJM+03, UTM+02, UTT+04, WLL07a, WDZs07, XLL+02, YLW+08, ZLLS06b, ZKZ+07, dOMSL01]. CH/
[MM05, OO08, SSS+09]. chain
[BHG03, DLW06, Der09, Dm00, ENM+04, GT03, HFHL06, JPF+00, KG02, Kr03, LL03a, LL01, MT03, PFC03, SMG09, TBC00, SWR06]. chains
[Cri04, CA07b, DLHC06, MMLC05, MSR04, VM02, XLT07, ZM06]. chair
[BP09]. chalcogena
[FKRE08]. Challenges
[KF02]. challenging
[BS06, NGTB03]. chameleonic
[PA05]. Change
[KIFK07, OFIK09]. changes
[HH04, JO02, Kar06]. channel
[CS09, FCP+04a, FCP+05, HSMT04, MCR08, RAGL09b]. channels
[DAK08]. chaos
[LSY02]. character
[ALC08, OV03]. characteristic
[YGZZ05]. characteristics
[DF06, KZY09, LZZC09, SLC+09]. Characterization
[FGR07, GGP09, GTC06, HYT05, HTSR04, DLW06, FDSA00, KHY00, LXL07, Mit01, SC01, TSMG01, YPNE09]. characterizations
[LS08a]. characterize
[Wou00]. characterizing
[PHJ+08]. Charge
[CM09, HT05, JK08, MZ05, SWM04, ZY01, BB05, BSP06b, Chi03, DWC03, ECM+03, FHR07, GY08, GDV03, GGLR00, GY06, GHBB04, HMOG07, IC08, JC09, JYVK09, KSO01, LFZS04, LLS03, OR05, PB04, PMB04, PP08b, PMPG05, RL05, RSN+02, SL09, San01, SKSH07, SH5F05, SRB02, SvDS01, TCT03, WSM+09, WM04, XL02, XLT07, YKO8, ZBS03, ZHO8, SDCG02]. charge-based
[HMOG07]. charge-density
[ECM+03, XL02]. charge-scaling
[YY06]. charge-transfer
[GGLR00, LLS03, ZHO8]. charged
[PPYS08]. charges
[BC+01, BCN07, CR09a, CGBF05, DVP+02, GHBB04, HS01, JLB00, JLB02, KGL07, KC01b, LMV07, PG06, SR09, TBSM09, TGGP+00, UBDP04, WMS06, XLT07, YOB+08, dSGCG00]. CHARM
[BBM+09, HLN08, HMD06, JKI08, LLL03, MM05, MMY07, PB04, PMB04, WHG+07, WRBV03]. CHARMm-based
[WRBV03]. CHARMM-GUI
[JKI08]. CHBr
[ZWL+05]. CHCl
[LDT+02a, ZLLS04b, ZLLS06a]. CHCLOHF
[YJWH09]. Chebyshev
[II02]. chelation
[TFZRG01]. Chem
[Bo01, HNF12, Kne05, KWK+00, Qua01, Van08, WHG+07]. Chemical
[BHTCG07, BBC+05, GC03, HLS07, JAC09, MGMM07a, PB07, PYCD03, PY05, WPS02, AM07, AGMR+08, ATH+03, CZFH07, CDD+02, CWWS07, DF06, DBS07, DA01, DPM09, DSS03, DMN05, Dra00, DWH+07, Fau01, FVB08, FR06, FLK+07, FK07b, FHF+01, FO04, GR07, GGB07a, GGB07b, GBB07, GS04, HFN101, HHP04, JHZ09, KF09, KFJH08, Kau07, KBL08, Koe03, KIM+09, KCO1b, KGD06, LWK08, LZZC09, LHP01, LDT07, LKA01, MA05, MC06, NRRK02, OH05, OHH+02, PPX01, PA08, PFC03, PG04, PHKG07, PC05, PC07, PRS04, PV07, RNG03, RM07, Rud05b, Rud05c, RSS09, RON02, SAM06, SM08a, Sch03, Sch00, Sha07.
SC01, SS05, SHH07, SFRS01, SCP08, TLOG00, Tru07, TT02, UNM+01, VBS09, VBGL+00, VKCK09, WS05a, WFHP01, WHP02, WWS07, WZXY07, XYN+06, ZB07, ZMH+09, HP05]. chemically [AVS09, Bud07, SB01, PP08b].

chemicals [CMGDAC+07]. chemisorption [KKJH08]. Chemist [SH08, Bic09, Gan09]. Chemistries [Duk01, EA08]. Chemistry [Ano05b, Ano06a, Ano06b, Ano06c, GBL+05, vRS98, WB04a, WWC+05, DBM03, FJP07, FKRE08, GDPCPU07, GDPP08, GdSuM+07, GdAcV+07, KSB+02, KBA+04, KJVW08, KYL03, KCO1a, LX07, MGCA07, MR09, MBP09, MMRVH07, MPF00, Nye07, SH07, Sha07, SBB02, SGD06, TKH07, Vis02, Ano01c, Ano04b, LB99, Lip00, Sta00].

chemistry-based [SBB02]. chemists [Pra01]. Chemometric [HPL03, MRS09]. chemometrics [BLF02]. chemotaxis [FC06]. CheY [UTT+04]. CHEFOCHF [YLWL09]. Chichester [Lip00]. chief [Lip00]. CHIMERA [NSU+02, PGH+04]. Chiral [ST04]. chlorated [DA01, WDZS07]. chlorinated [MDN05]. chloroform [CCK01]. Class [ZH06]. clathrate [EM03a]. clay [ATH+03, DJT08]. cleavage [CLXC02, DLL+09]. cleavages [XWXC08]. closed [SPT+03]. closed-shell [DSB+02]. class [CRK08, EBD+01, LL07, VIP+06, NYW05]. classes [CLF+09, KH06, QLHL09, XSHC06, XLC08, XWC09]. Classic [SRE08]. Classical [ATBLS04, COL+06, DK01, LLM09, MA05, Nil09, RP07a, STH02, Zho06]. classification [GDPCPU07, dGW01]. classifier [CLF+09]. clathrate [EM03a]. clay [ATH+03, DJT08]. cleavage [CLXC02, DLL+09]. cleavages [XWXC08]. closed [SPT+03]. closed-shell [DSB+02]. cluster [KRJ01]. closure [CSJ04, DLSVY00, Mak08, SWR06]. Cluster [AHKG09, CR04, BR04, BP01, BGJ01a, BWI+02, IN08, JBGK08, KJKH08, KSTC01, LM02, LWX07, LYS08, Mck07a, MS01, Mor02, NK06, PSF+08, SS07, VDB06, WKY01, Whe08, WJ+08]. cluster-continuum [WJX+08]. cluster/adsorbate [BW+02]. clustered [FPN+05]. clustering [CCWH02, FKF09, LZ05a, LOL+08, RL01, ZS04]. clusters [BP00, BACJCT01, CGG06, CAG07, DSX+02, GBH09, HX08, HY06, JMB+09, JMB+11, JG03, KGL07, KD+09, KZ+05, LML+00].
LWLS07, LJS05, Mck07a, Mck07b, NB04, OS03, OS08, PB00, Pul05, QB05, SCC04, SYC08, SW06, WLL01, WZZ+09, WCS09, XZ04, YCS07, ZLJ03, ZXL+04, ZWC+09, ZXY03, ZGXX06, ZX09, ZB07, Est07. CM1 [UBDPJ04]. CM3 [UBDPJ04]. CN [LW04a, TJM+03, TYN05]. CO [GD06, PLC08, RD00, TJM+03, VS02, KT08, ABYM08, DLD+02, FLK+07, PB00, SS05, PLC08]. co-ligation [KT08]. CoA [LLL+08]. coagulation [PDP02]. Coarse [CA07a, EBAN07, VTT+08, CP09, DR07, DJB02, HXL09, MBC08, PSHP08, SBJ08, WWL+09]. Coarse-grained [VTT+08, CP09, DJB02, HXL09, MBC08, SBJ08, WWL+09]. Coarse-graining [CA07a, EBAN07]. coastline [UTH+03]. cobalamins [KPZK06]. cobalt [LMIF06]. cocaine [ZDS+05]. cocrystals [CWV+05]. code [BDW00, FROD08, GBL+05, GJK+06, GY08, PZWG+04]. codification [CGMPT+08]. coding [LCSZ09]. coefficient [CSB+03, YSJ09]. coefficients [CCK01, DA01, GS09, Gol09, LZZC09, Whe08]. cobalamins [KPZK06]. cobalt [LMIF06]. cocaine [ZDS+05]. cocrystals [CWV+05]. code [BDW00, FROD08, GBL+05, GJK+06, GY08, PZWG+04]. codification [CGMPT+08]. coding [LCSZ09]. coefficient [CSB+03, YSJ09]. coefficients [CCK01, DA01, GS09, Gol09, LZZC09, Whe08].
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, HD0+02, HMK02, IV04, IvS06, Ish04, JH03, Kle02, KV06, LB05, LDL+09, MM03, MCF05, MY08b, MY08a, NH06, Pac06, ZWB09].
completeness [AHK02, MV06].
completeness-optimized [MV06].
Complex [DFGB09, AS06, Bac09, BRS00, BRS01, GC04, HDF+07, HD0+02, HMK02, IV04, IvS06, Ish04, JH03, Kle02, KV06, LB05, LDL+09, MM03, MCF05, MY08b, MY08a, NH06, Pac06, ZWB09].
complexation [AGI+07, HT05, LMMW04, SRK+00, SLRC01].
complexed [Pin03, SDM02, WCF04].
Complexes [APG05, AB00, Ano06a, ACM+06, BTP09, BR04, BL06, BM00, BGC07, BZ02, CG03, CBC+08, CSA08, CBH+03, DPT03, DF04, FRS05, FO08, FRLN09, FKS+09, GTC06, GL04b, GM01, GPS06, GPK05, Gni04, GZ09, GWO07, HLD06, HRG07, IO08, IGL07, JMD+02, JD09, JCHS07, KMA02, KJP+07, LL00, LHJ+06, LPH06, LH02, LMK06, LMS03, LMMW04, LWS09, LZF+09, LS05b, Mas04, MC08, MHS06, MSBS01, MLL+08b, NyHN06, NR04, NMAT01, PGG06, QTDG+08, RP07, ROPM01, RRFC+03, SG07a, SCF+09, SBH02, ST06, SV+08, TGGP+00, UM03, VS02, VMA03, VLO0, WB07, WWT08, Won09, ZY01, ZBS03, ZW+09, ZTS09, dBO01].
complexes* [GK09].
complexity [BT00, PK05, XSHC06].
Component [KBA+04, CCT+03, GP06, JMD+02, PVdB00, PV03, SH02, SM08b, Van02b, WG02].
Component-based [KBA+04]. Components
[SHC06].
Composition [HM06, KWH07, LL07, PAS08, XSHC06, XLC08]. Compound
[CN05, BR07, HBM06, RDO0, ZOX05]. compounds
[AACL03, BB08, BLO+02, CYM02, DA01, EBDPM00, ED09, EBD+01, FJ08, FROD08, FO04, G090, G091, JH03, KDF06, LLA01a, LLA01b, LLA01c, LLA01d, LLA03, LD05a, LW08, LT0+07, LWO06, LC03, LC03a, LJM+07, LMM09, MD04, NBN04a, PZ04, PZ04+04, PZ04+05, PO01, RUP06, SJJ+04, ST01, TTM09, YCW+09, YSA+03].
Comprehensive [LF02, Z009b, Z009b, DL+08, JF+00, SBL05].
Compression [BG07, MBW03]. Comprising [Rud05b, Rud05c]. Comput
[Bo01, Qua01, Van08]. Computation
[BLL+06, Car02, CDD+02, FZZL07, GOF09, LFE06, TNS00, AT03, G03, NK02, PAS08, RK05, WZY07, ZC03, vW06]. Computational
[An01c, An04b, An05b, An06a, An06b, An06c, BL08, C05, CP09, CMG09, CMGDA+07, CMG09, CG05, CA07b, GBL+05, GAPC07, GDS07, HM02, KLO+04, LB09, LIP00, MW00, MFR07, OY03, P06, SP08, vR08, S00, TMBM02, WB04a, WWC+05, WXX08, You11, ZOJ+06, ZWB09, Ba04, BG00, BAL+01, BTO09, BM00, BZ05, C05, CMS05, CFS+08, CBC+08, CJS+03, CRH+07, FG03, FJP07, FD03, FKE08, G090, GD09, GDP08, GG07a, KJ03, MCF07, M03, MH08a, OTL08, O01, OSA06, Pan07, P05, FW05, PRS04, RGG08, SF07, SM03, STJ08, TD08, Vi02, VZM+08, WSM+09, WOC+03, YT03, YT04, YD06, ZZ08, ZG07, ZTP+08, Z06, W001].
Computationally [K00, KF03]. Computations
compute \cite{BDW00, RKA09}. computed \cite{PFJ03, PK05, TDH06}. computer \cite{HFSD03, H505, NK01, PXXP01, PHJ+08, TRS02, UHHN09, VBO7, VKCK09, YNZ+08, Zer08}. Computing \cite{HHW+03, WL00, BHH+09, DGH02, DP04, DK01, GLD08, HHS+05, KBF05, LM03, MA09, ZP03}. CONAN \cite{SSHT03}. concave \cite{Won09}. concentration \cite{GGT08}. concept \cite{LSY02, Rao00b, Rud05a}. Conceptual \cite{VB09}. Concerning \cite{FG03, Bor03}. concerted \cite{LFS+07, Mck07b, NSB08, LLKC06}. condensed \cite{CLP09, DGI+08, DWC+03, FM00, GLMV09, Mor02, SDvG01, ZSK07}. condensed-phase \cite{DWC+03}. condition \cite{SK08}. conditions \cite{BVW04, CEP07, HH04, WM06}. Condon \cite{Ama02a, LMCD09, TP01b}. conduction \cite{SM06}. conductor \cite{DHW+00, FZL+06}. conductor-like \cite{DHW+00, FZL+06}. Configuration \cite{HS00, HHP04, KAS+07, DBM03, ENM+04, FWH+07, GB04, HDO+02, HP05, LKZ04, MW00, OFB08, OKH+02, PC00, PFC03, Rao09, RP09, TLKT00}. configurations \cite{NHH05, CLWL09, CIB05, yCkHmY08, DBM03, ENM+04, FWH+07, GB04, HDO+02, HP05, LKZ04, MW00, OFB08, OKH+02, PC00, PFC03, Rao09, RP09, TLKT00}. Conformation \cite{GS04, BY06, BR03, BLB09, DPM09, LXL07, PFJ+03, YL06, YZ06}. Conformational \cite{GS04}. Conformational \cite{AJNG01, AZS+04, BLF02, DSS03, HW09, KK09, LRI+02, LGB+09, OYK+09, OM04, PSMD00, SH09, SMGE08, SSHT03, SR09, TTB01a, TTB01b, WHRG08, WV04, BISB02, BMTSC01, BAH+02, CN03, CSJ01, CVG08, CS01, CCP04, CSRST04, CKT+08, DDKV07, DSR+07, ECA06, FGR07, FC06, FD03, GT03, GB09, HYA02, IB04, IZA06, JW06, JO02, KB02, KK08a, KH01, KE02, KK01a, KF08, LFKL00, LKJ+04, LCKL05, LJL08, MFB04, MAK08, MH08b, MA05, MGJAARC00, NKS02, OML+00, OGH05, PRT+07, PRT+08, SPL+02, SWBM08, SHBD05, SD09, SSBE06, WCK00, YXL+09, ZA07, CG03, HJCP01, JPF+00]. Conformations \cite{NHH05, CLWL09, CIB05, yCkHmY08, DBM03, ENM+04, FWH+07, GB04, HDO+02, HP05, LKZ04, MW00, OFB08, OKH+02, PC00, PFC03, Rao09, RP09, TLKT00}. conformers \cite{HS00, HHP04, KAS+07, PG01, RSSKB03, TT02, WD04, YXL+09}. Congo \cite{SRK+00}. Conical \cite{IK00}. conjecture \cite{Pog03}. conjugated \cite{BG00, CZ05, DDPB09, LYS08, LC09, LFR07, WJ00}. connectivity \cite{EDAJ04, Pog06}. conquer \cite{AKN07, MLJ03, vdVGDM00}. consensus \cite{GP06, JMD+02, LLL+08, RHL09}. Consequences \cite{RSS09}. considerations \cite{GRCD01, PB05}. Consistent \cite{RP02, BWI+02, ECM+03, KK08a, KBN02, NUH02, SMD02, VTT+08, WM04, XL02}. Constant \cite{MCM04, DRRM03, Sch00, Vas02, WLLS05, WLL+07b}. constants \cite{Cbo07, FCW06, GGB07a, GGB07b, HWFN01, JHZ09, KE03, MMLO05, MGL03, MDJ04, PJPJdPRM07, RRFC+03, SLL+04b, SFRS01, TLOG00, WDX+02, WZXY07, ZXY08}. constrained \cite{COS01, EC06, LFKL00, MM00}. Constraining \cite{AM09, HSWW00}. constraint \cite{BL09, FS98, FS00a, KvhGH01, YXC+07}. constraints \cite{BVW04, Bud07, 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 [BS06, FLOD07, FPN+05, JPF+00, LKJ+04, LWW+06, LFR07, LLM09, MSH+06b, PFC03, RRZA08, SL09, STC+08, WL04, Wil01b]. contemporary [CFS+08]. content [CLC03]. context [KMH02, KBT03, OCP02]. contexts [Sim07]. Continuous [FZL+06, LF04, LFZS04, ZFL+05, HHHS01, SM08b, PDC+08]. Continuum [FCP+04b, MGL03, ABWT09, BCIB05, CFR08, COL01, CCT+03, COL+06, FKL+06, FEVM01, FBLO08, GS02, GWS+02, HC08, HS01, HHP04, KKS04, LRI+02, LJ04, MLW+08, Pom04, RSP03, Sch00, STSF02, TJE03, VP09, WJX+08, YCBM00, ZFW08]. continuum-solvation [Sch00]. contours [YGZZ05]. contracted [GS09]. contraction [CGSdST06]. contribution [BCIB05, CR09a, DBS07, KC01a, LKA01, PWHF+03, PWHF+04, PMPGP05, RI07]. contributions [CBC+08, CR08, CSB+03, COL+06, GPK05, HIM07, MGL03, RM07, SWV+05]. Control [Kar06, DB06, LR06, MN02, RS05]. conventional [WMW03, WMW04]. Convergence [KGN07, LST08, GG09, LTV08, LJ04, Mas04, Rud05a, Rud05b, Rud05c]. convergent [PAS08, Zhao06]. Converging [GC04, KF02b]. conversion [CC09, CFD04, PHR+05, RR05]. converting [RM00]. Cool [BHG03]. cooperation [ATMK03]. cooperative [HLB09, RRCA08]. coordinate [BGC+09, HDBD04, Ish02, KTA03, LN01, RWBH09]. coordinated [GWL07, Sha02, SBH02]. Coordinates [EA06, Din00, EC06, GKK07, KU03, LPK07, NKS02, QCK01, QCK02, TNS00]. coordinating [JRJ01]. Coordination [KZRO03, Gor01, HXD08, SFR07, TBG00]. coordinations [DSB+02]. Cope [PA05]. copolymer [CHA+07]. copolymers [YFR05]. copper [CR02, DBS07, FNP+06, PMGL03, PBZ00, PS03, ZWC+09, ACM+06]. corannulene [Won09]. core [ATM+07, CM09, FR06, HXD08, HYR06, HJCP01, ION07, LFK05, LK03, LK04, NTH09, ON07, Pog03, TJM+03, TLKT00, TJE03, TKN+08, YCS07]. core-excitation [ON07]. core-excited-state [TKN+08]. Cornell [RKH03]. Coronavirus [LXZ06]. corrected [NTH09, PSC+01]. Correction [Duk01, CFC+08, GA106, Gri06, HK08c, HK08d, IKN08, LBT07, MGLS00, Mue01, QCK01, QCK02, SPD01, STSF02, TKH03, WX09]. corrections [BF07, Gri04, KSS08, WB07]. correctly [LF04]. corrector [Kol04]. correlate [Kle03]. Correlated [GBB07, BWW+08, BLT03, DBM03, GSP06, KMA+07, PF005, TBG00, WMW03, WMW04]. correlating [NSO+07, SNM+06]. Correlation [LRWG03, TDH06, AAP00, AGI+07, AS00, BL00, CKT+08, EL09, FDM00, GKT04, HN02, HR08, HI08, IKN08, JJK+00, JSH07, KGN07, KK08a, KC01b, LMJ02, Mat03, PJPdPRMI07, PMC+08, SRE08, TKB07, WMW03, WL04, YH09, dSGCC00, WMW04]. correlations [DR09, HHW+03]. Correspondence [RLRE01]. corrrhycene
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[NyHN06]. **COSMO** [EK06, ELK⁺09, KEH⁺02]. **COSMO-RS** [EK06, ELK⁺09, KEH⁺02]. **COSMOS90** [SO07]. **Coulomb** [WMW04, BWP07, Nee03, WMW03]. **counterions** [JD09]. **counterpoise** [GA06]. **counting** [HYT05, LM03]. **Coupled** [BSP06b, MO01, CXZ⁺09, DOSG06, IN08, KSTC01, LMJ02, LYS08, PSF⁺08, SSB07, WKYU01, Whe08, XWC09, SMAdV00]. **coupled-cluster** [IN08, KSTC01, Whe08]. **coupling** [CR08, DXW08, GdAcV⁺07, KTM02, KBLP09, LB08, MDI04, PJPdPRMI07, QtdG⁺08, Rl08, RL01D09, RRFC⁺03, SM08a]. **couplings** [BPC01, NR04, TP01b]. **CoV** [LZ05b]. **Covalent** [BSG07, BMTFR08, PML03, RS07a, RS07b]. **covalently** [PHFC04]. **Coverage** [SURG06]. **covering** [RKH03]. **COX** [WC09]. **COX-1** [WC09]. **COX-2** [WC09]. **CP** [ZKZ⁺07]. **CPHF** [ASWG07]. **Cr** [KPR04, Kri08]. **Crehuet** [Bof01, Qua01]. **Criteria** [Kle03]. **Criterion** [ALTB06, GLD08, PSDM00]. **Critical** [GT03, BMLV04, BLN01, BAÅ07, CRC⁺08, CKMC04, FMPS08, LFR⁺04, MP03b]. **Cross** [Gan09, MY08b, MY08a]. **Crosscorrelation** [HWDB03]. **crossed** [BAL⁺01]. **crossings** [LI07]. **crossings** [LSG06]. **crossover** [KRLD09]. **crown** [GLRL02, HDO⁺02, LWW⁺06, ZWY⁺09]. **crown-shaped** [LWW⁺06]. **Cryogenic** [HN02]. **Cryptand** [WWT08]. **Crystal** [KOFF09, Van02a, DPT03, EL09, HN02, KP05, TD08, VV08B02, vDSSvA04, vDSSvA03, vEMK01, vE01, DRMD03, FROD08, PZWG⁺04]. **crystalline** [AS00, CADW03, JB04, PZWG⁺04, Wil01a, ZLD09]. **Crystallographic** [RON02]. **Crystals** [BCF⁺09, CC07, FÁ01a, GAdGM08, GB03, PMC⁺08, RD06, WMS06, Wil01b]. **Cs** [GWL07, GLRL02]. **CSA** [NCO⁺05]. **CSOV** [GSP06, PMPPG05]. **Cu** [BTP09, GSP06, Shao2, HS08, NK06, TDK07, WMS09, ZTP⁺08]. **CuN** [ZX08]. **cuprates** [MDI04]. **Current** [NYTH09, CDPL09, Vis02]. **Curvature** [TRS02]. **Curved** [ABW09]. **Curves** [BBI⁺09, SM06, SSS⁺09, ZLY07]. **Customized** [BDW00]. **Cut** [BME05]. **Cutoff** [GG08T09, KL01⁺09]. **CuX** [KBL08]. **Cyanines** [BG00]. **Cyano** [PA05]. **Cyanoacetylene** [YDS06]. **Cyanobiphenyl** [CC07]. **Cyanoboranes** [WC08]. **Cyanomethylidynes** [WDS06]. **Cyclic** [KJP⁺07, BG01a, CLA⁺00, FK01⁺06, FK01⁺07, JB08, LXL07, OYK⁺09, VVS07, WOC⁺03]. **Cyclic-AMP** [FK01⁺06, FK01⁺07]. **Cyclization** [PWFS01]. **Cyclizations** [SG03]. **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]. **Cyclopeptidic** [FL07]. **Cycloreversion** [QZZZ03]. **CYP2A6** [VB09]. **Cysteine** [CN05, MOP⁺07, PPM06]. **Cysteine-6** [PMM06]. **Cysteines** [CFR06]. **Cytochrome** [AST06, ATBS04, HBM06, JKL08, LCC09, OYH05, OON01, ZAT07, BS06]. **Cytosine** [KKMMS04, MDOA08, MHS05, MI08a, SBI08, SG07a, SC01].
cytosine- [MHS05]. cytosine-5-acetic [MH08a]. CZ [CRC+08].

D [IS03, PF06, SHBD05, AGO+02, BAH+02, CPC+00, DDBP09, DMC05, FR0D08, GDPCPU07, GdSaM+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, SPM00]. Dead-end [YFS07, Adc04, GLD08, KUB07, SPM00]. deaminase [MDA08].

dearomatization [HT05]. debates [Nye07]. decarboxylase [HLC09, LLL+08]. decarboxylation [UTH+03]. decker [RPNJ07]. decomposable [VZM+08]. decomposition [BM07, CBH+03, FKO7a, FPG+06, Hir08, KZY09, KN04, LB08, ML00, SKD08, TBS09, TCR+02, ZZL04]. decompositions [GPS06, PBF07]. decoys [LZ05a, SRC03]. defect [ZMH+09]. defects [JT08]. Definition [EA06, LFSB03a, LFSB03b]. Definitions [PBF07]. Definitive [dOMSL1]. deformation [GHBB04]. 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 [SHH07]. delineate [MP03a]. delocalization [BY06, BI06, FVB08, FS02, Kar06, GMGM07a, GMGM07b, WMW03, WW03, WMW04, Wan09]. deltorphin [OM04, YAÇ+02].
deMon2k [GJK+06]. denatured [GB04]. dendrimeric [SCG04]. densities [GY08, GB03, HSWM00, KCK+08, LMV07, RLR+04, VZVG06, Van02b]. Density [BP01, FG02, Han01, JCHS07, KWK+01, KWK+02, MSBS01, QZZZ03, QZL+04, VL00, WCM08, AB00, ABYM08, AEE+03, ASY01, BAC09, BP03, BMLV04, BB08, BAÄ07, CLP+05, CRC+08, CKF06, CRS05, CR08, CSB08, CAG07, CPML08a, Cu04, CGSaST06, DVP+02, DVRP+03, DF04, ECM+03, FCW06, FZL07, FDM00, FS04, GHLK+02, GLRL02, Gri04, Gri06, GBHB09, GHBB04, HGBM04, HLS07, HNWF07, HNWF12, HN02, Hir08, Hol05, IO02, ION07, IN08, IB04, ITN+05, IS07, JNV08, Jac09, JCA+02, JFG04, KGL07, KRM+02, KN04, KSS08, Kle03, Kui00, KZW+05, Kri09a, KS01b, LRI+02, Lro06, LV08, LMB08, LMGR05, LLS03, LW06, LKT04, LF02, LLZL09, LDL+09, LZF+09, MP03a, MV09, MS00, NK06, NTH09, NAT07, OKE+02, PSF+08, RB01, RK04, RLER04b, RDM+08, RR05].
density [SLRC01, SSB07, SW06, TBG00, TST+08, TKN+08, TKH03, Van02b, VMA03, VBS09, VC04, VKCK09, WR+06, WB07, WZY04, WMRW+01, WL02, WCHW09, WM04, WCL05, WZXY07, WM01, XB08, XL02, XPW09, YTH01, YL09, YK08, YYW07, YLL+09, ZL04, ZH08, Zho06, ZM03, vGG00, Haf08, LWK08, MW00, XY+06, GM01]. density-functional [HNWF07, HNWF12, LLS03, LWH06, TST+08, XBN08, TKH03, Van02b, VMA03, VBS09, VC04, VKCK09, WR+06, WB07, WZY04, WMRW+01, WL02, WCHW09, WM04, WCL05, WZXY07, WM01, XB08, XL02, XPW09, YTH01, YL09, YK08, YYW07, YLL+09, ZL04, ZH08, Zho06, ZM03, vGG00, Haf08, LWK08, MW00, XY+06, GM01].
density/polarization [YL09].
deoxynucleoside [PFR04b].
deoxyribose [LBG08, SA07].
Dependence [ASS+02, MGLL03, BRLS08, BRLS12, BL00, KH06, NK06, SR09, TJM+03, VKCK09, ZP03, ZXY08, DvG00, DPM09, MG06].
dependencies [FHF+01].
dependency [OKH+02].
dependent [Bac09, CFK08, FCW06, FCP+04a, Gog08, GS04, HNWF07, HNWF12, HS01, ION07, LDY+08, LML+02, MW09, MY08a, NTH09, ONHN00, PF+08, TST+08, Whe08, WC08, YH07, ZH08, ZM03, vGG00, PM05]. depiction [ZTS09].
deposition [UNM+01].
deprotonated [Mas04].
derivation [EBD+01, JFG04, TT05, TTB+01a, EBD+01, HZ06a, Tor02, Tot04].
derivative [CNN07].
derivatives [BT00, BC06, CJK+02, COM+04, DMC05, DOS06, FL08, GLRL02, IS03, PSF+08, PA05, QCK01, QCK02, RP09, SPS08, SGPS09, Sch00, TSC+08, TNS00]. derived [GB03, HS01, Iw02, KS06, KF08, ML03, SvD01, TBM09, WMS06]. Deriving [RPMP03].
desaturation [BB06].
descreening [MM04].
describe [DDB09, IDM09, MSH+06b, RLD09, SB08].
describing [CML+04, HK08a, HK08b].
Description [ION07, MHT01, BUMCMRL00, BME05, CML09, CHRL09, GRI04, HGB04, SM08a, VMA03]. descriptions [SB08].
descriptor [CD09, RS09, TCSM03, XYN+06, ZNL07].
descriptors [AGMP+08, BA07, DA01, EDJ04, HM08, LMMS09, JG09, LHX+09, MGG07, RUP06, Tio09, TTB09, Wou00].
Design [AG03, KV00, BPS06a, BMTC01, BLMS08, CRH+07, CM08, DB06, DHW+07, Dhw09, GH03, Ham07, HM06, HLTL09, HLM05, JG05, LFBSK07, LZ05b, LFS+07, MWE02, NH05, PS09a, SPS08, SR07, SH04, STC08, VGG105, VZM+08, YFS07, ZZ08, ZL09]. designed [GT03]. designing [GD03]. Desirability [CM08].
desirability-based [CM08].
desolvation [HMOG07, SWV+05]. Detailed [PB05, WRB03].
details [GGB07a]. detecting [HH+09]. Detection [WHH+06, BAL+01, CMCB08, OYH09].
determinant [GS09].
determinants [BCT03, BCT04]. Determination [BLT03, CFR06, CR08, DLD+02, FSS00, Vas02, BL08, BR03, BCN07, BDPRMA100, CC09, CH03, CAGR08, FARG02, GCCV00, HP05, MA03, MG00, MM07, PC00, PFC03, PAB03, RI07, RTG00, SCF+09, TBS09, vDSS04].
determinations [YXL+09]. determine [DDV09, KUB07, OO08, RI08, YH06]. determined [OYH05, TDH06].
determining [BY06, DV02, LR06, PHJ08]. Deterministic [LS05a].
detonation [JWB05]. detoxification [ZWS09]. developed [CRS05, KMH02, RG08]. Development
[ATMK03, BGJ01a, HHJ03, IS07, KSB02, KOML08, KVL04, LAT05, LK03, MSR04, MRC03, WWC04, WWC05, WS05b, XYN06, Yan04, BA08, COS01, CMGDAC07, KLB03, NG04, BG03, IKYM09, SM08b].

developments [FCP04b, HS07a, SMD02]. DFT
[BRLS12, ASDP06, ACM06, BWP07, BPC01, BP07, BSB05, BM08, BB08, BE07, BRL08, BBSS06, BZL05, CMJ08, CCCJ09, CHA07, CG06, CS03, CMA08, DGD05, Der09, DDBP09, ESP04, EKO01, EBL08, FO08, FO04, FKS09, GCCVB00, GKH05, GPSP06, GKT04, HLLN06, HT05, HSWW00, HK07, HZ09, Hua09a, JPF00, Kle02, Kle03, KTM02, Kri09a, KPZK06, LMV07, LYK04, LWS07, LS08b, LWZ09, LS05b, MML06, MOP07, MGGO6, MBWP03, PFJ03, PMPGP05, PMM06, RM00, SBI08, SWB08, SBL05, SN06, SCS04, SSBE06, SRB06, Tle09, VS02, VB09, WMGK07, WLX05, WWT08, WJX09, XKG05, YS00, YK08, ZSE08, ZKZ07, ZWS02, ZWW09]. DFT-D [DDBP09].
DFT/MRCI [KTM02]. DFTB [ECM03].
di- [CU01, GBB07]. di-arsenic [KS05a].
diabetes [PS09a]. Diagonalization [LSAS01, BdPRMAI00, PU09].
diagram [Hir08]. diaminoguanidine [BI06].
diaminosilylene [TKS01]. diammineplatinum [DMN05]. diamond [EKO01, JBGK08, ZMH09]. diatomic [OSA06].
diatomic [ALKH04, FCW06, TLOG00, WWS07]. diatoms [Cul08].
Diatropicity [CdML06]. diazonium [EL06, EL07]. diborane [wQZsLyZ02].
dibromomethane [LXSF08]. dicarboxylic [NHH05].
dichlorides [LHP01]. dichloromethane [RRZA08]. dichroic [MM00].
dichroism [AB08, HKHN08].
dichroism [CDL06]. dihydro [WJX08].
dihydrodiol [PCMG09]. dihydropyridine [HC01a].
dihydroxypyridine [YXZ04].
dihydrophospholophole [CDL06]. dihydroxypyridine [HSMT04].
dihydroxyphospholophosphate [BY06]. dihydroxypyridine [YXZ04]. diinminobenzosemiquinonate [BA09].
diiron [BB08]. diketiminate [GTC06]. diketonate [RMP01].
dilute [HRR05, Kri09b, XZ04]. dilution [DA01].
dimensional [TSMNG01].
dimensional [BP01, Bie04a, CVR08, DHW08]. dilute [LR06, MP03a, MVLG06, RSS09, SHBD05, Wan09].
dimensional [CDGS09].
divide [AKN07, MLJ03]. divide-and-conquer [AKN07, MLJ03]. dizincocene [GXK09]. DL_POLY [KSY+00]. DMPC [HNL08]. DMS [RAGL09a, RAGL09b]. DMS-OH [RAGL09a]. DMSO [RAGL09a, RAGL09b]. DNA [AB08, AZM03, BCP03, DLW06, DLWW07, EL06, EL07, FPN+05, FKM+06, FMK+07, JMD+02, JCL05, LW04b, LD05b, LXX06, MB00, Maz01, PG04, Pin01, Pin03, PSHP08, PSS+04, PSMB05, RTG00, SG07a, SHD°08, WRP°06, WWP°09, hYDN°08, YS00, ZLY07].

DNA-base [PG04]. do [SRK°00, YJF06]. Dock [BS08, CWV°05]. docked [NMAT01, ZWB09]. Docking [BTLP03, RGZM09, WS02b, AGI+00, AGI+07, AB09, BS05, BS08, CMC04, CBC+08, CLH+07, CGBF05, CWV°05, CR09b, GZM09, HR08, HLM05, HW09, KG02, KCL06, LR03a, LCKL05, MKT04, MM03, MCR08, MHL°09, RK05, Ru07, SBG°09a, TH02, TGO04, TJE03, TP01a, Tot04, VVS07, WRBV03, YK00, Yan04, YKK09].

dodecamer [JCL05]. Does [RY09, RS07a, RS07b, WCK00]. DOIT [SFRS01].

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

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

DommiMOE [DFWH05]. Donald [Sta00].

donation [HT05]. donor [RM07, SEKS09].

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

doping [SM06, JBGK08].

dot [CLZ°09]. Double [LB05, AZM03, CMJ08, DLRR09, LMGO°09, Won09, YS00].

double-stranded [AZM03]. doubles [IN08, WKY°01, dSVA°09]. doubly [CHRL09, LDL°09]. doubly-linked [CHRL09]. Douglas [YH09].


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

Dramatic [AM06a, KT05]. dressed [MW09]. driven [MH09, PV03, SVT09, WPS02]. drives [LFS°07]. driving [AM07]. Drude [LLM09].

drug [CMCB08, DHW°09, HS07b, LLW°09, MCR08, PPX01, PFR04a, SPGS08].

drug-induced [CMCB08]. drugs [BLB09, KEH°02, KCOa, SMM°08, VGGM05, WM01].

DsbA [CFR06].

Dual [WyLG°09, WLL°03, ZWL°05, mLZL°07, TST°08, ZZL°04].

Dual-level [WyLG°09, WLL°03, ZWL°05, TST°08, ZZL°04].

Duan [Ano06c].

due [Car02, JM07a].

duplexes [BL08, NL08]. duration [CCS00].

during [IZA06].

dyad [CHRL09].

dye [BG00, KS05c].

dye-sensitized [KS05c].

Dynamic [SDCG02, XLZ08, CC07, CVR08, CEP07, FEV°09, JW06, mLZL°08, LW04a, LDG02, LEV°09, QCK01, QCK02, SDL°09, SCC04, SYC08, WM06, XLC08, YCS07, YCYX03].

dynamical [CKW09, EM03a, Kri09b, LDTS07, MS03, LPK07].

dynamically [CvG08].

Dynamics [BBG°04, DJB02, KB09, KIM°09, SSB06, Yos02, ALB09, ATMK03, AM06b, BL09, BB05, BWE05, BRDC02, BS01, BG07, CLP09, CL09].
CADW03, CW02, CIB05, CCSJ00, CF06, CPC04, CMD04, DLG00, DSS03, DBGV07, ES00, EMP07, ESM06, FSM09, FHRR07, FG02, FBDG06, FEVM01, FKK09, FPN05, GL04a, GL04b, GL05b, GS02, GO07, GSTD09, GJK00, HB09, HGMB04, HSWN01, HN02, HTSR04, HW03, HTN03, HLB09, Ike04, ITS05, ITS06, IC08, JS07a, JP09, JCL05, mJlZsLyL07, JHZ09, KMH02, KSB09, KM00, KM07, KSY00, KAK09, KZRO03, Kol04, KvGH01, KPR04, Kri08, Kri09b, Kro03, LLM08, LSG06, LGB09, LWY09, LR03b, Loe03, LMIF06, LM03, LPB03, MB00, MFB04, MN02, MM03, MABM09, MBC08, MCR08, MDA08, MOP07, MZK09, Kol04, KvGH01, KPR04, Kri08, Kri09b, Kro03, LLM08, LSG06, LGB09, LWY09, LR03b, Loe03, LMIF06, LM03, LPB03, MB00, MFB04, MN02, MM03, MABM09, MBC08, MCR08, MDA08, MOP07.

dynamics [Maz01, MVL05, MO09, MH08b, MCM04, MST08, MS01, NK01, NB04, NYK09, OO04, OO06, OR05, ON07, PMGL03, PRKP05, PMB04, PBW05, Pin01, Pin03, PZS04, PPYS08, PHH08, PHRR08, PB02, PNG08, QNF09, RRZ08, RMHK03, RG08, SO07, SH09, SJ08, SBG04a, SLL04a, SM03, STH02, Ste04, SDM02, TYN05, TLK00, TFN04, TK08, Tru07, UTH03, VSK04, VCM01, WCF04, WLLS04, WLL07a, WyLG09, WLL09, WEE01, WDX02, WLL03, XXL02, XLZ08, YLG06, YTH07, ZZL04, ZWL05, ZWS09, ZWZ09, ZSK07, SO07].

dynamics-quantum [ZSK07].

dynamics/order [MO09].
dynamo [FAB00].

E-state [SPGS08].
E1 [YT04].
E2 [RY09].
EADock [GZM09].
eyearly [CMCB08].
earth [JHMB09, JHMB11, SO07].
earths [LZZC09].
ECEPP [Sen06].
economic [FZL07].
edge [XWL09].
edge-doped [XWL09].
Edited [Sta00].
Editor [JW12, WM12, vLBBR12, Lip00].
editor-in-chief [Lip00].
Editorial [Bro05].
Editors [BFS07, FA01b, FB09].
educing [BS01].
Effect [CXZ09, CN05, CEP07, KGL07, Moe01, WMW04, BB08, CP00, CPJ01, CGB09, CSB08, CKT08, DMJ05, GT03, HK08a, HK08b, KT08, KMM07, KCL00, Kri08, Lee09, LL01, LCA03, Mas04, MZL08, PCS04,RY09, RR05, SO05, SPDS01, SCG04, SDL07, VM07, WM06, WDX02, XWL09, ZY01, ZZS07, ZWPR04, CPDH08, HFS07, JD09, WMW03, WSC09, vE01].
Effective [OCB02, SBLK01, VBGL00, BCF09, CR09a, DPT03, HMWC03, HSWW00, LFK05, MML02, NGTB03, NG04, RPM03, SG07b, VAS02].
effectively [SMGE08].
Effects [DXW08, KKH07, RLP08, XXWC09, AD00, ASS02, BA03, BA04a, BA04b, BPCA01, BE07, BDW00, BBI09, CC07, CK01, CDPL09, Don08, Dra00, ECA06, FGR07, FHF01, GMW08, GVAT03, GM04, GGLR00, GKT04, HRR05, IC08, JJK00, JW05, KSK00, LS08b, LR03b, Loe03, LFR04, MDA08, PBF09, PSF08, PWFS01, RRCA08, SF07, SL09, SMAD00, SURG06, SM06, SN06, SRB06, VMD06, WMGK07, WD04, Wib04, XY06, YXZ04, YH09, ZX04, ZWS02, CM09].
efficacy [KSM05].
Efficiency [IO08, MKGA06, RLR04a, YAC02, CN03, FSM09, GF08, KK08a, LJ04, LJS05, LW04, PSMB05, SM08b, SM03, SE08, vLBBR12].

Efficient
[AT02, BP00, BB05, CSJ01, DMZT08, EA08, FL08, FKZ09, GHH07, GB04, HMWC03, HTKG08, KMA⁺07, KCL00, Nil09, OD09, Oos09, SAT004, SSM08, TP01b, WM12, YZ04, Ami00, BL09, BP02, BdPRMAI00, CGG06, CIB05, CY09, CY13, DBS08, FG02, GJL⁺08, JBJB00, JJB02, KM00, LSO04, LCKL05, PRSM02, RKA⁺09, SAM06, SSMW09, TS05, Tot04, WW03, YXL⁺09, vLBBR12, FS98, FS00a]. efficiently [IGL07, LR06].

eigenvalue [SSL02]. eight [CWV⁺05]. elastic [AJ03, BED02]. Electric [LTV08, SF07, WMS06, ACD⁺03, BSOB05, CM09, Kar06, LST08, Mar03, OBBS05].
electrical [KCL00]. electride [LWW⁺06]. electrochemical [Bie04a, Bie04b, Rud05c].
electrocyclization [ZGZX07]. electrolyte [CCCJ09, YSJ09, ZCS04].
electron [AS00, BK08, BWW⁺08, BLN01, CFS03, FS02, Li01, OON01, PC05, PC07, TKH07, TD06, ZJM⁺07, AEE⁺03, ABF⁺03, BG03, Bac07, BG00, BY06, BMLVO4, BI06, BRS07, BL00, BAÅ⁺07, CRC⁺08, CXZ⁺09, CR09a, CHRL09, CHT⁺08, DVP⁺02, DRVPR⁺03, EL09, FLOD07, FR06, FS04, FZL⁺06, FSS00, GKR08, GGA00, GR07, GBJ03, HLS07, Hr08, HSWW00, IK08, ITN⁺05, IS07, IN01, Jc09, KS05a, KK08c, Kle03, KFD06, Kri09a, KMMMS04, Lai07, LMV07, Lee09, Leh06, LV08, LL01, LLS02, LH02, LB05, LBG08, MLL06, MGCA07, MGMM07a, MS00, MA09, OKE⁺02, PFB05, PA05, PAS07, QZZZ03, RS07a, RS07b, RTG00, SFC04, VC04, VKCK09, WMRW⁺01, Wan09, WL00, XWXC08, Yas08, YCXY03, YH09, ZXL⁺04, PC05].
electron-correlation [YA09]. electron-pair [FS04]. electron-repulsion [Kri09a].
electron-sharing [BRS05]. electron-transfer [QZZZ03].
electron/four [GYMN07]. electronegativities [dSGCG00].
electronegativity [ALC08, BCN07, JVK09, VK06].
electronic [CWWS07, DNM⁺03, FLK⁺07, GGGL05, Hua09a, IME02, KHY00, KMM07, KGD06, LPP06, LTF⁺07, OS08, QB05, RPNJ07, SCP08, Wu06, WWS07, XZ05, AJ03, AEE⁺03, Am02a, AZS⁺04, AGSFA⁺05, ASS⁺02, Bac09, BBG⁺04, CMAGL⁺04, CZFH07, CN05, CNG07, CRBS03, CSV⁺07, CTFC08, DD00, FL08, GJL⁺08, GBL⁺05, GM04, HMMS09, HZ09, Hua09b, Kar01, KR⁺02, KP⁺07, KIHK07, KWK⁺00, Kri09a, KPZK06, LWK08, LWS07, LWZ09, LFR07, LB08, LDF⁺09, LMRVFH⁺09, MKGA06, MM02, NYH02, PP08b, PMC⁺08, QCK01, QCK02, RRC08, RS05, SSB⁺03, SBL05, TD08, TT01, TD06, TDK07, WMRW⁺01, WL⁺05, W00, YXY⁺04, YFR05, YSS0, ZZ07, ZFS⁺07, ZYY08, ZXYF09, XZ08, ZL05, ZL07, ZL09b, ZM03, SMKM00]. electrons [HIM07, Pog03, WJ00]. electroosmotic [YSJ09].

electrophilicity [RUPH06]. electrophoresis [WW⁺09].

Electrostatic [CCT⁺03, GYM07, PK05, PML03, RLER04b, SG07b, ABWT09, BCN07, CPUG09, CHMI05, DWNB01, FOL⁺04, GY06, GPK05, GBJ03, KFZ03, KLH⁺04, KCK⁺08, MMPK01, PMB04, PP08b, RLP08, SMA00, SSS05, VGSU08, VC04, WCK00, YH06].
electrostatics [HS01, ML03, RSP03, STSF02, VVBV02, WMS06, ZFW08].
electrototopological [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 [BWW+08]. ELIA [BWW+08].

elimination [Adc04, CF03, 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, CUY02, FM00, Gri04, GGK+08, HRRB03, JCHS07, KK08b, LRM09, MB00, RKK03, ZNLI07, VBGL+00].

employing [MHT01, THHN01]. empty [CZA03]. enantiomerization [Qua07].

Encapsulated [WL09b], enclose [ZBS03]. Encyclopedia [vRS98, Lip00]. end [Adc04, GLD08, KUB07, PSDM00, YFS07]. endohedral [KSN01].

Endoperoxide [BLO+02, CG08].

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

Energetics [KRLD09, AHGK09, DBGV07, Hua09b, ILKR09, LD05a, MFB04, Mas01b, MOP+07, SDCG02, WSC09, ZXY03, ZX09, DLG00].

Energies [CRSB03, BP02, BWE05, BLL+06, BE07, BDW00, CHA+07, CCK01, CPML08a, CG05, DB07, DZMT08, FOL+04, FJ07, FKU+05, GS04, GKT08, H05, HYA02, Hol05, IIO08, JJJ+09, JACL05, JZD+09, JG03, JSHG07, JCHS07, KKW+01, KWK+02, KSTC01, KCO1b, LN01, LSW+01, LFEDL06, MT03, Mas04, MLL+08b, NHH05, PK05, PSF+08, RSS03, RSE07, RSN+02, RM00, SZT08, STSF02, SYC03, SA07, SLRC01, TKS+01, UBDP04, Var09, VC04, WCK00, WLX+05, WSS05b, WW04, XLT07, ZMM09, ZW09, ZM03, vGGB00].

Energy [CBH+03, HFFH06, IN08, KLS02, MSF+08, NKO6, SSB07, WM12, dSR08, AMR04, AJ03,ABA04, AE06, AM06b, ABBC01a, ABBC01b, AGSFAL05, BM07, BCB05, Ber03, BL05, Blo04, Bo01, BLRS08, BRLS12, BACJCT01, BF07, BLB09, CC09, CN03, CCB04, CY09, CY13, CJW+09, Chi03, yCkHnY08, CV09, CMGAD+07, CA04, COL+06, DLD+02, DLZ09, DMBV05, DK01, EGSG00, FSS09, FK07a, FJK+01, FZL+06, GZL02, GMA04, GLMV09, GadGM08, GG09, GC04, GS02, GS03, GS06P06, GB02, GWS+02, HKMS01, HP01, HRO8, HMOG07, IGH03, ILKR09, IGL07, IPN06, IPN07, Jac09, JMJ+02, KGN07, KN04, KKK05, KUB07, KB09, KOB03, KCO1b, Kri09a, Lab08, LR03a, LMK01, LF04, LFZS04, LJ04, LG08, LKW04, Lu09, MG06, MCF05, MAF+07, Maz08, MH09, MGJARAC00, MGL03, MRS+07, Nak02, NKIS02, NA06].

energy [OD09, OFB08, ONHN00, OKH+02, OV03, Oos09, PSC+01, PMGL03, PK04, PAT+09, PMPGP05, Qua01, RP07a, Rap00b, Rap06, RES07, RRE08, RWBH09, RHL09, SOOF05, SPDS01, SKGS00, SPL+02, Sch03, SMGE08, Sen06, SRCD03, SSM08, SY09, SG07b, SSMW09, SMD02, SJW09, SSBE06, TJE03, TGGP+00, TCR+02, UTH+03, VE09, VM02, Vya01, WL02, WD04, Whe08, WHF08, XZZ04, YXC+07, YZ04, YHD+06, ZCZ03, ZZ08, ZGXX06,
vEMK01, vLBBR12, Hir08. Energy-based [KLS02, MSF+08].
energy-consistent [SMD02]. energy-transfer [MAF+07]. energy/one
[Oos09]. energy/one-step [Oos09]. enes [PWFS01]. engine [MVL+05].
Enhanced [KG02, DAK08, NYTH09]. enhancement [AB08].
enhancements [AM06a]. enkephalin [ZCL09]. enones [SLRC01]. enough
[VGGMM05]. Ensemble [Blo04, BSC+01, EMP07, O06, SM08b, SM03].
ensembles [GLD08, Ike04]. enterovirus [KCL06].
Enthalpies [EB04, WC04, BE06, BSJ01, Hir08, NTH00, SBB02].
enthalpy [OVMV04]. entire [ZAT07]. entropic [CBC+08, FGR07].
entropy [DHF+05, HDF+07, HTKG08, KKH+07, LM03, RK05, Ruv07,
STSF02, WG02]. enumeration [AL01]. Enveloping [BHH+09, CV09].
environment [DFWH05, DPM09, GT03, HFS+07, PMM05, GBL+05].
environmental [CMGDAC+07, FGR07, MDA08, TP01a, VW03].
environmentally [EDAJ04]. environments [MP00, ZFW08]. enzymatic
[PCM09]. enzyme [CFER04, Fie02, GGLR00, GS04, MDA08, Pin03, TDH06,
VB09, ZL09a]. enzymes [BS06, CPUGD09]. enzymic [CG05, TCR+02].
Epimerization [BBSS06]. Epitope [SHBD05]. epitopes [KVS+06, SHBD05].
epoxide [Owe05]. epoxides [YO03]. epoxy-amine [YO03]. EPR
[SN06]. equalization [BCN07, JVV09, VK06]. equation
[AMR04, ABWT09, BHW00, BH03, BF04, BF07, BRS00, BRS01, FS00b,
Höf05, HBW00, HBW01, SAT04, TW03, Vas02, Vis02, Zho06]. equations
[Bie04a, CF04, DSG06, Har04, Kvh01, LPK07, LMJ02, QNF09, RTO7,
Rud05a, Rud05b, Rud05c]. equilibrated [CA07a]. Equilibration [SDCG02].
Equilibration-Morse [SDCG02]. equilibria [FGR07]. equilibrial
[Kli01]. Equilibrium [KSTC01, BBP09, ECA06, KBLP09, LS08b, MMLC05,
PAS08, ST04, WMMK07]. EQUIPATH [Kli01]. Equivalent
[ZZY07, WBS03, ZZY08]. equivalents [RCJ02a, RM00]. ERE [MCF07].
Erratum [ABBC01a, Ano05b, Ano06a, Ano06b, Ano06c, BA04a, BRLS12,
CY13, FS00a, HNVF12, HBW01, HK08a, JHMB+11, KW+02, LFSB03a,
LR03b, NBTN04a, PCO+07a, PWHF+04, RS07a, TZX01b, W04a, W05,
WMW04, WWC+05]. error [IO08, KMA+07, Kob03, Mas04, MD04, RS05,
Rud05a, Rud05b, Rud05c, TBS09, VKP+08]. error-ranked [TBS09].
errors [CS03]. erythronic [vDSSa04]. ESFF [SYY+03]. Essay
[BHTCG07, FKO7b, GR07, Kut07, MGCA07, Nye07, Shao07, Sim07, Tru07].
established [SB01]. ester [TH02]. esters [POJ01]. estimate
[KC01b, YZ04]. estimated [ZMZ09]. estimates
[GS04, HT05, MD04, SY09]. estimating [HDF+07]. Estimation
[DH07+05, ZW09, CV09, DDVD09, HLTLP09, KC01b, PYEA03, Lab08].
estimators [GZL02]. estrogen [FKU+05, KBK+01]. ethane [DGD+05].
ethanes [WyLG+09]. ethene [Ang09]. ether
[GLRL02, WD04, WLL+03, YLW+08]. ethers
[AELD03, LCDA03, LCGA03, LCA03, ZYW+09]. ethyl [KH+07].
Ethylene [TBG00, BSJ01, Hir08, NTH00, SBB02]. Euclidean [RRS09].
EUDOC [PPXP01]. Euler [SG01]. evaluate [GGB07a, GGB07b, LF04, OSH03, TSSGS07]. evaluated [ABBC01a, ABBC01b, Bo01, Qua01]. evaluating [FO08, Con02]. Evaluation [BMLV04, DR07, KSM05, NMAT01, OYH09, VKP+08, YSJ09, Ano05b, AGSFAL05, CGG06, CAG07, DSR+07, DBS08, ESP04, FMAMVK06, FKZ09, GGA00, HMWC03, JSHG07, KJVV08, KH06, LMV07, LYS08, MSH+06a, Mor02, PRS04, Sha05, VP02, WL02, Yan04, Yas08, CBC+08, GKT04, OGH05, ZSK07]. evaluations [SF05]. Evans [SRK+00]. EVEBAT [CZA03]. Even [CVVB04, CC07, VVBV02]. Even-tempered [CVVB04]. evidence [BLO+02, IO08, SFR07]. Evolution [BMLV04, DR07, KSM05, NMAT01, OYH09, VKP+08, YSJ09, Ano05b, AGSFAL05, CGG06, CAG07, DSR+07, DBS08, ESP04, FMAMVK06, FKZ09, GGA00, HMWC03, JSHG07, KJVV08, KH06, LMV07, LYS08, MSH+06a, Mor02, PRS04, Sha05, VP02, WL02, Yan04, Yas08, CBC+08, GKT04, OGH05, ZSK07]. evaluations [SF05]. Evans [SRK+00]. EVEBAT [CZA03]. Even [CVVB04, CC07, VVBV02]. Even-tempered [CVVB04]. evidence [BLO+02, IO08, SFR07]. Evolution [BMLV04, DR07, KSM05, NMAT01, OYH09, VKP+08, YSJ09, Ano05b, AGSFAL05, CGG06, CAG07, DSR+07, DBS08, ESP04, FMAMVK06, FKZ09, GGA00, HMWC03, JSHG07, KJVV08, KH06, LMV07, LYS08, MSH+06a, Mor02, PRS04, Sha05, VP02, WL02, Yan04, Yas08, CBC+08, GKT04, OGH05, ZSK07]. evaluations [SF05]. Evans [SRK+00].
Extending [GCD04, MFB04]. extensible [SYY\textsuperscript{+}03, GBL\textsuperscript{+}05]. Extension [CR09b, FBL008, GY08, TBGRJ04]. Extensive [JW12, LB08, SLHW09, YXL\textsuperscript{+}09, ZL05, SMG09]. external [CM09, EC06]. extra [LW07], extra-valence [LW07]. Extracting [HM02], extraction [OD09]. extrapolated [KSTC01, Var09]. extrapolation [MO09, MC06, PSC\textsuperscript{+}01, PFJ\textsuperscript{+}03]. extremal [ZZ08]. extremely [GFS05].

Eyring [Nye07].

F

[CR\textsuperscript{+}08, FO04, Gog08, HYA02, HZ09, Hua09a, IV04, KS05a, KBL08, Mar03, RB01, STC\textsuperscript{+}08, UTT\textsuperscript{+}04, WLLS04, WLL07a, XLL\textsuperscript{+}02, ZY01, ZLLS06b, ZL09b, HK07, KS05a, RFSS06, SOOF05, Sha02, WDWS06, WYHZ03].

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

Fast [JBJB00, JJB02, JSHG07, NG04, RS08, SYC03, SFC04, Ami00, ATMK03, An05b, CS02, CRG01, CHMI05, CZA03, GY08, GKK07, HH04, HLM05, Isg04, KLM\textsuperscript{+}09, KvgH01, KH06, PZS04, RK05, San01, SCC04, Sha05, TRS02, VPO2, WCC08, HC08, LZ05a, VLH\textsuperscript{+}05].

faster [SF05, AM06a]. faujasite [TLOG00]. faujasite-type [TLOG00]. FB [DHW\textsuperscript{+}09]. FB-QSAR [DHW\textsuperscript{+}09]. FBP28WW [PAT\textsuperscript{+}09]. FDS [TJE03]. Fe [BTP09, HLLN06, HYR06, KRLD09, AGK03, KT08, DF04, Mck07a, Mck07b, NyHN06, NHN06, PLC08]. feasibility [MWE02]. feed [SJJ\textsuperscript{+}04]. feed-forward [SJJ\textsuperscript{+}04]. feedforward [LJZ\textsuperscript{+}07]. Felix [Ano06a, Ano06a].

FeMo [Mck07a, Mck07b]. Fermi [Kri09a, PYCD03, PYS05, PC07, PLC08]. ferrocene [Kan07, MBP09, ZZS\textsuperscript{+}07]. ferromagnet [TD08]. ferromagnetism [SK08]. FeS [Mck07a]. Feynman [RLER07]. Field [MO01, AS06, ACLD03, An06b, An06c, ATBL04, BWI\textsuperscript{+}02, CLP09, CLLL09, CPM03, CM09, CGB03, CLA\textsuperscript{+}00, CR02, CSU05, DvG00, DPT03, DRMD03, DFWH05, DMLI05, DGI\textsuperscript{+}08, DHW\textsuperscript{+}08, DWC\textsuperscript{+}03, EBD\textsuperscript{+}01, FHHRO7, FBGD06, FAR02, FM00, GZL02, GMA04, GRO\textsuperscript{+}03, GGK\textsuperscript{+}08, HP01, HGM04, HXX09, HIM07, HNL08, HMOG07, IDMC09, IT03, IKYM09, JS07b, JCL05, JM07b, JFG04, KB02, KSB\textsuperscript{+}02, KS06, Kar06, KFHN08, KTA03, KOFF09, KLB03, KYT\textsuperscript{+}08, KOML08, KDSV02, KVL\textsuperscript{+}04, KBN02, LL00, LST08, LTV08, LFZS04, LAT05, LH05, LLM09, MTO3, MB00, MM05, MP03b, MBC08, MMMY07, MRS04, MRC03, MHJS06, NUH02, NCO\textsuperscript{+}05, OYH05, OMHN08, OHHN00, OKH\textsuperscript{+}02, OVMV04, OBT09, PBO4, PMBO4, PS09b, PWHF\textsuperscript{+}03, PWHF\textsuperscript{+}04, POM04, PHH\textsuperscript{+}08, PJO01, PBO5, RSN\textsuperscript{+}02, RKH03, SF07, SO09, SDL\textsuperscript{+}09, SDvG01, SAS05]. field [SDCG02, SSS\textsuperscript{+}09, SYY\textsuperscript{+}03, SHK\textsuperscript{+}05, SP05, SK05, TAS07, TTB01a, VSW\textsuperscript{+}03, VCM01, VTT\textsuperscript{+}08, WK01, WWC\textsuperscript{+}04, WWC\textsuperscript{+}05, WZW\textsuperscript{+}06, WMS06, Wol01a, Wil01b, XLT07, YCYX03, ZWC\textsuperscript{+}09, vDSSvA04]. field-based [DMLI05]. field-derived [WMS06]. field-induced [CGB03]. fields [ABA04, Car02, EBD\textsuperscript{+}01, HRBKB03, LLM08, Mac04, MFB04,
OSHS03, PK04, PB02, RP07a, RLER04b, 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, Be04b, BF04, DRMD03, Der09, GM04, HBW00, HBW01, KG06, PZ04, RP07b, Rud05a, Rud05b, Rud05c, VZM+08]. finite-chain [Der09]. finite-difference [Bie04a, Bie04b, Rud05a, Rud05b, Rud05c, VZM+08]. finite-temperature [KGD06]. First [CS01, HZX04, Hua09b, TK08, WZZ+09, WD08, ZDS+05, ZXY09, ZHWM09, AD00, BP03, CK+02, EBL+08, FO08, GJL+08, GD09, JPC08, KK08c, LW09, Luk07b, MLJ03, Rud05b, VP08, WLX+05, XWL+09, KSB+02]. First-order [Rud05b]. First-principle [ZDS+05, GJL+08]. First-principles [CS01, HZX04, Hua09b, TK08, WZZ+09, WD08, ZXY09, EBL+08, GD09, WLX+05]. first-row [AD00, BP03, K03]. fixed [HM06]. fixed-composition [HM06]. Flex [GCD04]. flexibility [BL08, BCP04, KG02, KTA03, MHL+09, OV03]. Flexible [COS01, NGTB03, YK00, AGI+00, AGI+07, AJ03, AHGK09, BZP09, BTL03, BS08, CCL06, CMK04, CLH+07, DDV07, GCD04, HW09, JNO8, KOFF09, MH08b, SSBE06, TFN04, TP01a, Tot04, VLH+05, vEMK01, v01, TJE03]. flexible-backbone [AHGK09]. flexible-ligand [HW09]. flexible-protein [HW09]. Flooding [LSG06]. Fluctuating [OR05, KMH02, PB04, PMB04, Yos02]. Fluctuation [MH04, PC05, SBLK01]. fluctuations [AZS+04, WMGK07]. fluid [BCIB05, CLC09]. fluorene [CHA+07, YFR05]. fluorene-pyridine [CHA+07]. fluorene/carbazole [YFR05]. fluorescence [CHA+07, MAF+07]. fluorescent [DHM+03, NAT07, VSW+03, XZ05]. fluorides [BSG07, IV04]. fluorinated [KS05a]. fluorinated [CSU03]. fluorenebenzene [ZTP+08]. fluorobutanal [NSB08]. fluorocarbons [JARM02]. fluoroglycine [HS00]. fluoromethylene [ZLLS04a]. flux [DAK08, RKA+09, Rud05a, Rud05b, Rud05c]. fly [KMA+07]. FMO [FOK+04, FKL+06, KIM+09]. FO [Gog08]. focal [KK08a]. Fock [RRS07, TW03, WMW04, AK07, BO09, CU10, DD00, GAD08, HDBD04, MS00, MBWP03, PFT+03, PVdJ00, TYO+02, UHH09, WMW03, Wei08, YH07, vDSS+04]. Fock/Kohn [RRO+07]. Focus [Mat03]. focusing [KBK+01]. fold [DB06, ZM06]. folded [CP08, GB04]. Folding [HEP+02, ADM+06, CCC03, DG00, HG08, IM06, JS07a, JI09, KH05, MLG04, MHO9, MEI02, MWE02, RP09, RLP08, VW00, VW04, VGO+07, Z03, dSR08]. folds [BS01, Z04]. following [DLL+02, LMO09]. For-Gly-NH [PC00]. For-L-Ala-NH [PC00]. Force [CLP09, JCL05, OMM08, OBT09, SO09, SL09, ZWC+09, AM07, AS06, ACL03, AB04, An06b, An06c, ABTL04, CLW09, CAR02, CPM03, CLA+00, CR02, CSU05, DG00, DGI+08, DWC+03, EBD+01, FBDG06, FAR02, FM00, GRO+03, GGF+08, HP01,
ILKR09, IGL07, JZD+09, KDG+09, KAS+07, KKC05, KUB07, KB09, Kob03, KK01α, Lab08, LR03a, LF04, LSW+01, LKW04, MG06, MT03, MGLO03, MRS+07, OD09, ONH00, OKH+02, OV03, OVMV04, Oos09, PK04, PAT+09, RSE07, RBWH09, SOOF05, SAM06, SKGS00, STSF02, SBL05, SSM08, SY09, URDP04, UTH+03, VHL+05, VE09, VGSU08, VM02, WHF08, XLT07, YZ04, ZMZ09]. free-base [SBL05]. Free-energy [JMD+02, AM06b, CY09, GMA04, ONH00, RBWH09, SKGS00].

Free-energy-driven [MH09]. freedom [DHF+05, MZL08]. freeze [BME05].

freeze-and-cut [BME05]. frequencies [BRV+07, Han01, Kle03, KBN02, LMB08, PZWG+04, WM04, ZWPR+04]. frequency [DF06, DR09, My08a, VSW+03, YH07]. frequency-dependent [MY08a, YH07]. friction [JS07a]. frozen [AEE+03, GWS+02, JNV08]. frozen-density [JNV08]. fructose [MRS+07]. fuel [CCCJ09]. Fujitsu [KSY+00].

Full [PRSMV08, GD09, IR03, KGD06, RS08, ZCZ03]. full-atom [RS08]. fullerene [CHR09, CTFC08, GYCZ04, GKX09, Kan07]. fullerene-dizincocene [GXK09]. fullerenes [GZ07, GM01]. Fully [GW+00, XZZ04, WTKM06]. function [Bac04, BS05, BdPRMAI00, CFS+09, Che01, yChHmY08, CPUGD09, Con02, DMZT08, DP03, FSS00, GCB03, GS09, GaAcV+07, GPN01, HMWC03, HZ06a, HZ06b, ILB03, ILKR09, Ish04, KK08c, Kni00, KFD06, LR03a, LHI09, LBT07, MP03α, MLA02, MY08b, Nak07, NKIS02, PP08b, PA05, PAS07, SFC04, SJW09, TLKT00, TW03, TJ03, TT05, TSSGS07, VVS07, YLL+09]. functional [AAP00, AB00, ABYM08, ASY01, Bac09, BF01, BE09, CLP+05, CFK08, CRS05, CR08, CSB08, CPML08a, Cul04, DVRP+03, ECM+03, EL09, FCW06, FZL07, FG02, GHLK+02, GM01, GLRL02, Gri04, Gri06, GBBH09, Ha08, Han01, HNWF07, HNWF12, Hol05, ION07, IB04, ITN+05, IS07, JFG04, JCHS07, KGL07, KS08, KKW+01, KKW+02, KZW+05, Kri09a, LRI+02, LW08, LMB08, LMR05, LLS03, LW06, LKT04, LF02, LLZL09, LDL+09, LZF+09, MW09, MSBS01, MW00, NTH09, NAT07, OKE+02, PSF+08, PU09, PDS01, QZZ00, ZL+04, RB01, RK04, RDM+08, RR05, RZWS07, SH07, SZT08, SPT+03, SPT07, SLRC01, SS07, SW06, TBG00, TST+08, TK08, TKH03, Van02b, VMA03, VL00, VB05, WRP+06, WB07, WZY04, WM04, WL02, WCW08, WCHW09, WM04, WSC09, WCL05, WXYZ+07, WM01, XYN+06, XB08, XWC09, XLO2]. functional [XPW09, YYY07, YLL+09, ZL04, ZH08, Zho06, ZM03, vGGB00].

functional/continuum [LRI+02]. functionals [BP03, DF04, Han01, ION07, JPCA08, KR04, QZZ00, ZL+04, RB01, RK04, RDM+08, RR05, RZWS07, SH07, SZT08, SPT+03, SPT07, SLRC01, SS07, SW06, TBG00, TST+08, TK08, TKH03, Van02b, VMA03, VL00, VB05, WRP+06, WB07, WZY04, WM04, WL02, WCW08, WCHW09, WM04, WSC09, WCL05, WXYZ+07, WM01, XYN+06, XB08, XWC09, XLO2]. functional [XPW09, YYY07, YLL+09, ZL04, ZH08, Zho06, ZM03, vGGB00].

functions [AE06, Bac07, Bao00, CG03, CGSdST06, DVP+02, GFS05, GLD08, GS07, GB03, IT03, MLL06, MY08a, NUH02, OFB08, PFB05, RHL09, Ru07, SS05, TS05, TD06, WG02, YH06, ZM03]. Fundamental [LMB08]. fungal [LPP06]. funnels [HEP+02]. furfural [COMR+04]. Further [GPK05]. fusion [CRG10]. fuzzy [ALTO06, EKB02a, RLA01]. FVII [PDP02].
glucans [PCS04], glutamate [FTL01], glutamic [ZZY07], glutamine [WC08], Gly [PC00, VKP+08], GLYCAM06 [KTY+08, SDL+09], glycaminide [LB05], glycine [BA03, BA04a, BA04b, GAIMVB01, GS09, GKT04, KAS+07, LB05, LSW+01, MOP+07, PG01, ROG00, ZW09], glycol [Pin01, RR05], glycol-lesioned [Pin01], glycosidase [BMTFR08], glycosidase-inhibitor [BMTFR08], glycosidase-substrate [BMTFR08], glycosidic [SO09, SDL+09], glycyl [KOML08], going [CCK01], gold [BR04, CZ05], gold-capped [CZ05], GolP [IDMC09], good [VGGMM05], GPCR [XWC09], Gradient [SE07, DLD+02, DSR+07, FRLN09, GMA04, ION07, Ish02, IPN07, LST08, TNS00, WL02], gradient-based [FRLN09], Gradients [WM12, BWP07, HHS+05, IK00, KBT03, LJ04, SSMW09, vLBBC07], graphite [BCF+09, EKO+01], Gravitational [WS02a], greedy [TGD05], green [DHM+03, XZ05, KK08c, KFD06, ZM03], grey [XLC08], grid [ALB09, CG06, Pom04, RSN+02, RKA+09, SKSH07, STH02, WL00, WRBV03, YK08], grid-based [ALB09, RSN+02, RKA+09, SKSH07, WL00, WRBV03], GridMAT [ALB09], GridMAT-MD [ALB09], grids [Bie04a, SFC04, THHN01], GROMACS [KVF+07, LSG06, VLH+05], GROMOS [CLWL09, CHB+05, LH05, OVMV04, SHK+05], GROMOS96 [SDGV01], groove [BCP03], grossular [ZWTP+08], Ground [HM01, PO03, PSS+04, BBI+09, CYW09, FCW06, FDSA00, IR03, KRT09a, LMK01, ZOJ+06], Ground-state [HM01, KRT09a, LMK01, ZOJ+06], group [ATTLS04, CQ04, DVR+03, EL07, EB04, JWB05, JGH00, KBT03, LW07, MBM+00, MA05, RCJ02a, RZWS07, RKK03, SGPS09, SN00, TD06, dSGCG00], groups [BE09, EB04, FJ08, Van02a, WSC09], growing [QUI07], grown [WHH+06], Growth [TDK07, HMK02], Grubbs [YXC+07], Grubbs- [YXC+07], GS [MH09], GS- [MH09], GTO [CGB03, RLRE01], guanine [EL07, GWL07, HHWG08, JM07a, KKMM04, MSBS01, MHS05, SSMK00], guanine- [MHS05], guanine-cytosine [KKMM04], guest [LMMW04, Oos09], GUI [KIKI08, SD09], Guide [SH08, Woo01, You11, Bic09], guideline [MWE02], H [AGI+07, BAL+01, BPC01, BL00, CPJ00, CS01, DRAS04, GPSP06, HYA02, IN08, IS03, LDMM01, LMK01, LLXS02, LW04a, LYZ+08, LM009, Mas01a, Mas01b, MGLL03, SLL+04b, TYN05, UCT+03, WDXS06, XDS06a,
ZZL04, ZZZ+06, dRLMS00, CPDZH08, CJW+09, CGB03, DLD+02, Don08, EdlVR+03, Gog08, HK07, ITS06, LC07, LDC+07, LLXS02, LB05, LN01, LLL07, LS05b, LMO09, MR02, McD08, MY08a, NL08, OO04, PGRRRN03, PRSMM03, PV07, RFSS06, RRBH09, SOOF05, SEKS09, SLL+04a, WDS06, WTKM06, Wll08, Wll10b, WDX+02, YTY07, ZY01. H-bonded [LB05, McD08, NL08]. H-NMR [AGI07]. H5N1 [DLRZ09]. Hairpin [ZHH09, CJW+09, IGNH03, 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]. halo [TT02]. halo-hydroxymaldehyde [TT02]. haloacid [NYK+09]. haloalkane [CS03]. halogen [BS03, FHF+01, GGP09, LZF+09]. halogen-bonded [LZF+09]. halogenated [STC+08, TZX01b, TZX01a]. halogens [TBGRJ04]. halothane [TZX01b, TZX01a]. Hamiltonian [FGR07, FGb08, MR02, SAM06, ZWP+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, Bou00, GAdGM08, MS00, MBW03, PFJ+03, RRS07, WMW03, We10, YH07]. HAsXH [LS08a]. having [WJ00]. haystack [BS01]. HBCC [BAL+01]. HBOP [OYH09]. HBr [SL+04b]. HBSITE [OYH09]. HCCX [Mar03]. HCI [BL06, WDS06]. HCO [JPF+00, dRLMS00]. HCO-L-SER-NH [JPF+00]. HDRM [LRW03, LAR+03, LSHR04]. head [HSWN01]. heart [TKH07]. heartland [Sha07]. heat [dOMSL01]. heats [CS03, JWB05, RCJ02a, WX09, LLA01c]. heavier [ZJM+07]. heavy [BPC01, SLO9, 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, LJO7, PP08a, YS00]. Hellmann [RLER07]. hemagglutinin [DLRZ09]. heme [ATBS04, 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, YA+02]. herbicidal [XYN+06]. hERG [MCR08]. Hess [YH09]. Hessian [KK01a, NKIS02]. Hessian-free [KK01a]. Hessians [ASWG07, CNU07]. heteroaromatic [LLM09]. heterobimetallic [RD00]. heterochiral [ZOJ+06]. heterocycles [FSS00, MGMM07b]. heterofluorones [CZFH07]. heterogeneity [HS01, ZSC05]. heterogeneous [FCK+08, ZCS04]. heterolicenes [LC09]. heterolevel [EA08]. heteropentalenes [CDL06]. heteropolymers [SBJ08]. Heuristic [DMC05, DLM06, CAGR08, IZA06]. Heusler [GD09, KGD06]. hexadiene [PA05]. hexadiyne [PWFS01]. hexagonal [BK08, LTF+07]. Hexahelicene
[LC09]. hexamer [NK01]. hexatrienaldehyde [ZGZX07]. hexopyranose
[GGK+08, LH05]. hexopyranose-based [LH05]. HF
[BRLS12, BRLS08, FJK+01, GKT04, PMPGP05, WW03]. HF/6 [FJK+01].
HF/6-31G* [FJK+01]. HF/DFT [BRLS12, BRLS08]. HF/MP2
[GKT04]. HFCO [JHPRSM+05]. Hg [GPSP06, BB+09, WTKM06]. HH
[CMàGL+04]. HI [KKJH08]. Hiberty [Bic09]. hidden
[FWH+07, HL+05, RP07a]. hierarchic [RRS07]. Hierarchical
[LMH+09, CWV+05, DJB02, FOK+04, LCC09, UHN09]. High
[BB08, GAdGM08, LAR+03, AZM03, BACJCT01, CWW02, CN05, DPT03,
GL04a, GY08, HGMB04, JBB00, JJB02, KW+00, KVF+07, LR06,
Mck07a, Mck07b, MTB09, RP07c, RLER07, RSS09, SSS+09, WMRW+01,
WS05b, XK08, UTM+02]. High-dimensional [LAR+03, LR06, RSS09].
high-latency [KVF+07]. high-level [WS05b]. high-performance
[CC07, LR06, RSS09]. High-precision [GAdGM08]. high-quality
[JBJB00, AVS09, BWE05, CLXC02, DLG00, KWF+00, KVF+07, LR06,
Mck07a, Mck07b, MTB09, RP07c, RLER07, RSS09, SSS+09, WMRW+01,
WS05b, XK08, UTM+02]. High-resolution [GL04a, WMRW+01]. High-spin
[BB08, DPT03, Mck07a, Mck07b]. high-valent [AZM03, CN05]. higher
[BdPRMAI00, LMGR05]. Highly [ZFW08, BWW+08, CKMC04, CLH+07,
PPYS08]. Hildebrand [BBG+04]. hindering [HFSD03]. HINT [CPUGD09]. Hirshfeld
[DVP+02, DVRP+03, GHBB04]. histogram [Kob03]. histogram-based
[Kob03]. HIV [AJNG01, AVS09, BWE05, CLXC02, DLG00, KF08, NLL+09,
SPT+03, SVV+08, VVS07, WHF08]. HIV-1
[AJNG01, AVS09, BWE05, KF08, NLL+09, SPT+03, VVS07, WHF08]. HLA
[KVS+06, WCF04]. HLA-A*0201 [WCF04]. HLA-DQ2 [KVS+06].
HLA-DQ2/DQ7 [KVS+06]. HMLP
[DMC05, DLHC06]. Hoboken [Bic09]. hOGG1 [Pin03]. hole
[Li01, SZW+05]. hole-particle [SZW+05]. holes
[PYCD03, PYS05, PC07, PLC08]. homoalanine [MM00]. homochiral
[ZOJ+06]. homocoujugation [MMLC05]. homogeneous [FCK+08, Pog03].
homologous [CC07]. homology [KCL06, KVS+06, O08, SGS03, YKK09].
homopolyptides [JS07b]. homotops [TDK07]. Hongxing
[Ano06c]. HOO [BL06]. Hoover [QNF09]. hormone [HMK02]. host
[CS01, LMMW04, O09]. host-guest [O09]. Hou [JW12]. HOX
[WLLS04]. HP [VGDSU08]. HP-lattice [VGDSU08]. HSAB [PRS04]. Hua
[JW12]. Hückel [Kut07]. human
[FKU+05, HN01, HMK02, LCC09, PDP02, VGDSU08]. LX [RB01]. Hybrid
[BF04, HTN03, WR+06, ZSK07, AAPP00, BG00, BBSS06, DNM03, DDBP09,
FAR02, FAB+00, FMSA06, GRO+03, GLD08, HIBH00, Han01, ION07,
JPCA08, JIK09, KR+02, KN04, LSO04, LWZ09, LS05b, MBM+00,
MSh+06a, PDS01, RDM+08, Sza08, THIN01, TFFN04, WWL+09, XZL08,
ZZL04]. Hybridized [SJJ+04]. hybrids [GXX09, Kan07]. hydrate [IME02].
hydrated [ITS05, XZ04, YSJ09]. hydrates [EM03a]. Hydration [BZL05,
CFC+08, HN02, BLL+06, CMD+04, GZL02, HB09, HKMS01, HM02, Lab08,
LSW+01, MS03, NTH00, OVMV04, PK04, Pin01, RP03, UBDJP04, XLT07].
hydration-parametrized [RSP03]. hydrazines [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09]. Hydride [GVATG03, JHH01, LLXS02]. hydrides [KS01b, SBR06, dSGCG00]. hydridotris [HT05]. hydridotris [BLN01]. hydrazone [Lu09].
[Bor03, GTC06]. **imipenem** [SDM02]. **immune** [WCS09]. **immunoglobulin** [Kró03]. **IMOMO** [VM00]. **IMPACT** [BBC+05]. Implementation

[AKN07, CKW09, DRMD03, KBT03, LI07, PZS04, RNG03, SVT09, YTH+07, BMRDB01, BLMS08, DFHW05, DBS08, FROD08, GY06, JNV08, NBJ04, PZWG+04, SAM06, SM08b, TT01, VK06, WCC08, YCXY03, LLL03, VW03, YOB+08]. **implementations** [FL08]. implemented [HP01, MP03b]. implementing [OR05]. Implications

[AKN07, CKW09, DRMD03, KBT03, LI07, PZS04, RNG03, SVT09, YTH+07, BMRDB01, BLMS08, DFHW05, DBS08, FROD08, GY06, JNV08, NBJ04, PZWG+04, SAM06, SM08b, TT01, VK06, WCC08, YCXY03, LLL03, VW03, YOB+08]. **implementations** [FL08]. implemented [HP01, MP03b]. implementing [OR05]. Implications

[AKN07, CKW09, DRMD03, KBT03, LI07, PZS04, RNG03, SVT09, YTH+07, BMRDB01, BLMS08, DFHW05, DBS08, FROD08, GY06, JNV08, NBJ04, PZWG+04, SAM06, SM08b, TT01, VK06, WCC08, YCXY03, LLL03, VW03, YOB+08]. **implementations** [FL08]. implemented [HP01, MP03b]. implementing [OR05]. Implications

[AKN07, CKW09, DRMD03, KBT03, LI07, PZS04, RNG03, SVT09, YTH+07, BMRDB01, BLMS08, DFHW05, DBS08, FROD08, GY06, JNV08, NBJ04, PZWG+04, SAM06, SM08b, TT01, VK06, WCC08, YCXY03, LLL03, VW03, YOB+08]. **implementations** [FL08]. implemented [HP01, MP03b]. implementing [OR05]. Implications

[AKN07, CKW09, DRMD03, KBT03, LI07, PZS04, RNG03, SVT09, YTH+07, BMRDB01, BLMS08, DFHW05, DBS08, FROD08, GY06, JNV08, NBJ04, PZWG+04, SAM06, SM08b, TT01, VK06, WCC08, YCXY03, LLL03, VW03, YOB+08]. **implementations** [FL08]. implemented [HP01, MP03b]. implementing [OR05]. Implications
initiated [RAGLL09b]. initiation [GGGLL05]. initio
[AJ03, Ama02a, Ama02b, Ano06b, ASY01, BG03, BG00, BL08, BSB05, BS01, BL06, BLO+02, BSJO1, CJP00, CPM03, CUS00, CU01, CUS03, CLO09, CYM02, CJW+09, CHRL09, DGD+05, DWS+09, DPM09, DB06, Dra00, EM03b, FG02, FAR02, FO08, FNP+06, FKU+05, FKM+06, FKS+09, GKRG08, GD06, GBB07, GGLR00, GKTS04, GPK05, GBBH09, Ha08, HS08, HYA02, HELM09, HMSM06, HFHL06, HS07a, HTSR04, HSWW00, HJCP01, ITS05, ITS06, JCA+02, JFG04, JCHS07, KSB+02, KP05, KFNH08, KKG+09, Kle02, KF02a, KIFK07, KWK+00, KPR04, Kri08, Kri09b, LMK01, LYK04, LDC07, LMCD09, LMB08, LZJ03, LWLS07, LKT04, LF02, LXS08, LLL07, LZF+09, LMO09, Mar03, Mas01a, Mas01b, MDA08, MLL08b, MM02, MS00, MA09, MG00, MLC01, MW00]. initio [MS01, Mor02, ML00, Mui05, NYK+09, OO04, OON01, OS08, ON07, OO08, PP08a, PGN03, PGR03, PHRR08, RSSK03, RSE07, RRA08, ROG00, RGG08, SS00, SG07a, SAS05, SBL05, Sha02, SLL+04a, SSS+09, SRE08, SMK00, SMZW05, SK05, SSBE06, TAN07, TYN05, TZX01b, TZX01a, TGGP+00, TFZRG01, UCT+03, UM03, UTM+02, VSK+04, VS02, VIP+06, WMGK07, WLL07, WLS04, WLS05a, WOC+03, WDD+02, WXX03, WCL05, XL+02, YXC+07, ZSE08, ZZL04, ZZZ+06, ZW09, ZGXX06, ZX08, ZWTP+08, ZL09b, vDSSV04, vEMK01, vE01, CSV+07, MDI04, SH07, TBG00], inner [Pog03]. inner-core [Pog03]. inorganic [CMA+08, SYY+03]. inserted [BL08]. Insertion [ZVZ03, RD00, TBG00]. insight [MDA08]. Insights [BTP09, PSHP08, SBG+09a, MCK05, PAS07, SGS03]. instabilities [DD00, VW06]. instability [LPK07]. instead [Lab08]. insulator [RDM+08]. insulin [ITN+05, KVS+06, ZM06]. insulin-B [KVS+06]. Integral [JCA+02, BR00, BS01, CC09, CFD04, DBS08, GWM08, JF09, KJVW08, Lab08, MBW03, SVT09, UKN04, Vya01, Yas08, PVdJD00]. integral-driven [SVT09]. integrals [ABB+03, FL08, FMAMV06, FR06, GAA00, Ish03, Lai07, RLR04a].

integrand [GC03]. integrate [MP03a]. Integrated [BBC+05, HTO3, LOL+08, MS01, VKCK09, VM00]. integration [BK00, Bio04, CLF+09, ESP04, HTO3, JCA+02, KBA+04, LRWG03, Pom04, RP07b, SY09]. integrations [PFB05]. integrator [CF06, KM00, TNF09]. intensities [WKY01]. Intensity [Tor02]. Intensity-carrying [Tor02]. Inter [HRBKB03, MAF+07, RP02, SWV+05]. Inter-phyocyanin [MAF+07]. interacting [RG08, YCX03]. Interaction [BE09, GBBH09, LSAS01, MHS05, ROG00, AKN07, AB04, AZM03, BRLS08, BRLS12, CLO09, CF04, CFC+08, CPM08a, DLD+02, DMZT08, FK07a, FL07, GDD03, GWM+00, GS04, GKT04, HZO6a, IDM09, Ish03, KN04, KBT03, KSO5c, LDMR01, LIW07, LP03, MLL06, MN02, Mas04, NTH09, Oos09, PPXP01, PMPGP05, PRSM02, PRSVM08, RRA08, SS02, SYC03, SWZ04, SLRC01, TIK03, UTM+02, VC04, WS05b, ZC03, ZWP08, EB04, JCS07, LFZ04].
Interactions [CPML08b, FKŠ⁺09, Van08, ALC08, AG00, ASDP⁺06, ATMK03, Ano05b, AS00, BPC01, BM07, BUMCMRL00, BSJ01, CMaGL⁺04, CEP07, DDBP09, EFQD09, FA01a, FO08, FNP⁺06, FKM⁺06, FKM⁺07, GGP09, Gon07, HLC09, HA04, HZ06a, HZ06b, IINK09, IB04, JWB05, KF02b, KH06, LHJ⁺06, LCC09, LZJ03, LS08c, MM05, MMLC05, MCF07, NK06, Nil09, PG01, PCO⁺07b, PCO⁺07a, PK05, PNG08, RZW07, SOOF05, San01, Sha05, SS⁺09, SWV⁺05, SG01, SL06, SDL07, SMV⁺09, UTT⁺04, VW03, WR⁺06, WPH⁺07, Won09, YT03, YTH⁺07, ZTS09]. interactive [DFGB09]. interactively [SB01]. Interatomic [RD06, AMR04, SS00, SPT07]. interconnected [SB08]. Interconversion [OO04]. interconversions [FD03]. Interesting [Kri09a]. interface [CW02, DPDG05, FOK⁺04, GKRG08, HHBH00, HZX04, JKII08, KKG⁺09, LLL03, LPB03, PHJ⁺08, SMW04, 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, IGHH03, MMMY07, OBT09, WSM⁺09]. Intermolecular [PSC⁺01, AS00, CMaGL⁺04, CLC09, FA01a, FKM⁺06, FKM⁺07, GGP09, GS04, IGL07, KS05c, LZ03, Mas04, PMPGP05, RRA08, SPDS01, SJW09, UT⁺02, UTT⁺04, WI01a, WI01b, ZDS⁺05]. Internal [EA06, BHH⁺09, CFD03, CFD04, COM⁺04, DHF⁺05, Din00, HSDF03, KS03, KTA03, LPK07, SWR06, TNS00, WRS07, WFR08]. internal-rotation [DFH⁺05]. interparticle [PK05]. Interplay [EFQD09, SP05]. interpolated [YK08]. interpolation [BB05, IS03]. interpretation [CPJ00, HLS07, VM07]. intersection [SSHT03]. intersections [IK00]. interval [LS05a]. interwall [ZZvRSC08]. Intra [FA01a, FKM⁺06, FKM⁺07, MAF⁺07]. Intra- [FA01a, FKM⁺06, FKM⁺07]. intra-phycocyanin [MAF⁺07]. Intramolecular [GKTS04, HA04, PG01, TFZRG01, AGK03, BA03, BA04a, FDSA00, HRBK03, HK08a, Li01, NH05, RP02, SWV⁺05, VKP⁺08, VIP⁺06, ZDS⁺05, ZW09, ZH08, Kle02]. Intraprotein [MLJ03]. intraresidue [IB04]. intrinsic [JS07b, JT08, YGZZ05]. intrinsically [NAT07]. Intruder [CWY09, WCFH02]. intuitive [PP08b]. invariant [Est07, ZLY07]. Inverse [BR03, MLL08a, NI09]. inversion [KSTC01, RC04, ZSE08]. investigate [DWN01]. investigated [HN02, Kle03, YH09]. Investigation [LZZC09, YTH01, AST06, BLO0, CW02, CHA⁺07, CG08, GS03, GS04, Hr08, JH01, KFYF07, LH02, LXS08, NS08, PV07, QZZZ03, QZL⁺04, RM07, RC04, RO09, SL04, TGGP⁺00, TFZRG01, UCT⁺03, WL09b, WL⁺07, ZXY08, ZKZ⁺07, ZHM09, ZGX07, GB03, JBGK08]. Investigations [JP09, WG02]. involvement [BLO⁺02]. involving [LL01, MM05, ZGX07]. iodides [CM09]. iodine [GWM⁺00]. iodobenzoylphosphonate [GWM⁺00]. Ion [DAK08, BM08, Dra00, EL07, FHR07, FL07, GWM08, Gor01, IvSV06, KPR04, Kri08, Kri09b, MSBS01, PPS08, PHRR08, RC04, VHR07a, VHR07b, ZZW09, dOMS01]. ion-pair [RC04]. ionic [Ang09,
ionizable [OS06]. ionization [GSB09, KFD06, RTG00, SVT09].
ionospheric [LSHR04]. ions [CXZ+09, DMJV05, EL06, FG03, HTSR04, HLB09, JRJ01, KT08, KZRO03, LSWB00, LMIF06, MHS05, RMP01, SL09, ZSC05, ZZZ+06]. IPR [GZ07].
IR [NRKH02, ZWTP+08]. iron [DPT03, GK09, HLLN06, LWH06, MSH+06b, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06].
iron-containing [MSH+06b]. irregular [ZBS03]. irrelevance [VVBV02].
Iso [GWL07]. isotopic [GWM08, WDX+02, GM04]. isotopologues [LMB08]. isotropic [BCIB05].
isozymes [WC09]. issues [Mac04, PHFC04]. Iterative [PU09, Rao00b, CC09, HZ06a, HZ06b]. itinerant [SM08a]. IV [AZM03, CN05, CDL06, DMN05, FZL+06, LLA01c, LLA03, LCA03].

J [BPC01, Bof01, HNWF12, Kne05, Qua01, Van08]. Jacobi [IR03].
Jacobians [SWR06]. Jahn [Kri08, VDM06]. Jason [WB04a]. Jersey [Bic09]. Jicun [JW12]. jk [SPGS08]. JNK3 [KK01a]. John [Ano04a, Bic09, Lip00]. Joint [RP07d, DF06, PA05]. Jones [CYM02, FSK05, Pu05, SCC04, SYC08, YCS07]. Journal [Ano05b, Ano06a, Ano06b, Ano06c, WB04a, WWC+05, Ano01c, Ano04b].
journey [PSCD+09]. jun [KK01a]. junction [DWNB01]. Junmei [WWC+05].

K151 [NYK+09]. Kenny [Sta00]. Kepert [RMP01]. kernel [BR00, BRS01, DDV09, TSSG07, TSSG08]. kernel-based [DDV09].
etene [MG06]. ketones [LLA01a]. key [HEP+02]. Kick [AM09]. Kier [SPGS08]. Kier-Hall [SPGS08]. kinase [FCP+04a, FCP+05, GdSuM+07, HLT+05, HW09, KK01a, PB06, SWV+05].
kinechannel-phosphatase [FCP+05]. kinase-specific [HLT+05].
kinases [SWM04]. kind [LX07]. kinematic [CSJD04]. kinematics [LLC03, LFKL00, ML08a]. kinematics-based [LFKL00].
Kinetic [mJZsLyL07, Bie04b, BZL05, GWM08, Jac09, Kri09a, WDX+02]. Kinetics [CUS00, ST04, Gog08, HSL05, MG06, NSU+02, RLP08, UNM+01, VW00, VW04]. kinking [BCP03]. Kirchhoff [YOB+08]. Kirkwood [KS06].
Kirkwood-Buff [KS06]. Kneller [CSD05]. knowledge
[Adc04, HZ06a, HZ06b, LWW+06, NMAT01, dSR08]. knowledge-based
[Adc04, HZ06a, HZ06b, NMAT01, dSR08]. Kohn [RRS07, Bon00, SH02].
Kollman [JVK09]. Kr [CMJ08, CGB03]. Kroll [YH09]. Krylov [Har04],
krypton [CVVB04].

L [Bac09, HT05, JPF+00, PC00, AGO+02, HT05, HJCP01, KOML08,
NYK+09, OYK+09]. L-2-haloacid [NYK+09]. L-captopril [AGO+02].
L-2-haloacid [NYK+09]. L-2-phenylalaninamide [HJCP01]. L-valinamide
[HJCP01]. La/SSB [KVS+06]. 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].
lanthanides [RD06]. Lanthanum [AB00]. Large
[WCF04, ARL01, AB08, AS00, BG03, BP01, BdPRMAI00, BME05, CJK+02,
CDD+02, CG06, DMN03, DJB02, Elh07, FZL07, HB09, HSM06, IME02,
IS07, JO02, JW00, Ks05b, KKG+09, KK01a, KH06, LMJ02, MKGA06,
MH09, MW04, MH08b, MPF00, ME06, NRK02, PFJ+03, RRS07, SYC08,
SSL02, TY0+02, VSK+04, WWL+09, YCS07, vGB00, WS07].
large-amplitude [KS05b]. Large-scale
[WCF04, DMN03, JO02, KK01a, MH09, MW04, MPF00, ME06, RRS07, SSL02, TY0+02, larger
[VKP+08]. lariat [ZWY+09]. laser [Sha02, KZW+05]. latency [KVF+07]. latter
[LPK07]. Lattice [OCH05, SG01, HP01, KWK+01, KWK+02, KF02b,
LJK08, MH08a, SCC04, SYC08, TK08, VGDS08, YCS07, vE01]. law
[Sch00]. LCAO [EBL+08, EL09]. LDA [RLD09]. lead [RS07a, RS07b].
leads [PPXP01]. learning [YC+09]. least [CSD05, Go09, LLZL09].
least-square [LLZL09]. LEDO [GKH05]. legacy [Sha07]. Lei [An06c].
length [CRC+08, DR09, JPCA08]. length-frequency [DR09]. lengths
[PSC+01]. Lennard [CYM02, FSFK05, Pu05, SCC04, SYC08, YCS07].
Lennard-Jones [CYM02, FSFK05, Pu05, SCC04, SYC08, YCS07]. lesion
[Pin01, SHD+08]. lesioned [Pin01, Pin03]. Letter [BFS07]. Letters
[JW12, WM12, vLBBR12]. level [BUMCMRL00, BLT03, BL00, DPM09,
JMD+02, mjLizLyL07, Kk08c, PFJ+03, RC04, TBG00, TST+08, UTM+02.
WyLg+09, WS05b, WILL+09, Z LG+05]. levels
[BACJCT01, Cu04, DJB02, PFJ+03, WW03]. Lewis
[BHTCG07, GR07, Sha07, Sim07]. LF [PWHF+03, PWHF+04]. Li
[CRC+08, GBDP05, JW12, HDO+02, LWK08, LWL+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, BMTSC01,
CBG+09. CLH+07, CN05, DFWH05, FO08, GZM09, HZ06a, HZ06b, HWO9,
JZD+09, Ks08, LWH+09, Mue01, Rm07, NMAT01, OFIK09, PWHF+03,
PWHF+04, RK05, Ru07, SOOF05, STFS02, TFN04, TJE03, VGGMM05,
XZZ04, YK00, Yan04, ZGFL01, ZWS+02, BDW00, HLC09. ligand-charge
[BSP06b]. ligand-protein [VGGM05]. ligands
[BS05, CKMC04, FO08, FKI+05, GTC06, GM01, GGLR00, JFG04, RGG08,
SWM04, TP01a, TGGP+00, WS02b]. ligation [KT08]. light [Kr03, LFR07].
light-emitting [LFR07]. ligin [PS09b]. LiH [McD03]. like
[BCIB05, DHI+00, DB02, FZL+06, JD09, Kut07, LAEL01, PRKP05, WL09b].
limit [MV06, MLL+08b, PSC+01, SAS05, Var09]. limitations [BYQS03, LFEdL06,
PRDS08, MFB04]. limited [Ano05b, Sha05]. Limits [OV03]. line [RHL09].
Linear [Con02, DLWV07, KDG+09, LMJ02, OS06, OFIK09, SKDO08,
vdVGDM00, AT02,ABA04,BH03,BPCD07,CC09, CGMPT+08,GCDL+05,Gol09,
GGLR00,Har04,KLM+09,MW09,McD08, Oos09,PK05,RI07,RS05,SSB+03,
TCR+02,vGGB00]. Linear-scaling [OS06, SKDO08, GGLR00, TCR+02].
linearized [ABWT09]. link [GdAcV+07, KS02b]. linkages [SDL+09]. linked
[CMD+04, CHRL09, FS98, FS00a]. LiPF [BSJ01]. lipid
[HNl08, RGG08, SSM08, WC09]. Lipkowitz [Stao0]. 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
[HDX08, LWLS07, RC04, SLRC01, YSA+03]. liver [CMCB08].
LMO [BY06]. Local [Din00, LYS08, AGSFAL05, CPML08a, Ion07, IS03,
JHPRSM+05, KMA+07, LMJ02, MA09, PMC+08, RUPH06, SL09, SEKS09,
SB08, TT05, TSSSG08, VKCK09]. localizability [BK08, BW+08].
Localization [Che01, ALTB06, FS02, FSS00, GBJ03, PPOb6, PA05, PAS07,
PC05, PC07, SFC04, ST01, WMW03, WW03, WMW04, SHBD05].
Localized [ABF+03, AB09, Bac04, Bac05, Bac07, BME05, FMSA06, GFS05,
ITN+05, TT01]. locally [TYO+02]. locate
[ABB01a, ABB01b, Bo01, GMA04, MP03b, Qua01]. locating [WSM+09].
Log [Tot04]. London [Lab08]. Long [RP07c, CCSJ00, CPC+00, CEP07,
CSRST04, Gr06, KSS08, LYS08, MN02, MBC08, RLP08, San01, VVB02].
long-duration [CCSJ00]. long-range
[CEP07, Gr06, KSS08, MN02, RLP08, San01]. long-time [CPC+00]. lookup
[Nil09]. loop [CSJD04, KK01a, Mak08, OFB08, PRT+07, PRT+08, TLK00].
loops [CSRST04]. LoProp [SKK+07]. Low [DPT03, MG06, AG00, BS05,
GS03, KUB07, KK01a, KK01b, LAR+03, LB08, LB08, PFO+03, PRSMV08,
Rao00b, Sha02, WSO2b, 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, WSO2b, BS08]. lowest [FDSA00, OSA06, XZ04, ZL04].
lowest-lying [FDSA00]. ip [LAR+03]. Ip-RS-HDMR [LAR+03]. LR
[ZW09, NSO+07]. LR-MMPBSA [ZWB09]. LSCF [FA02]. Lu [SNM+06]. luminflavin
[CNN07]. LUMMOWX [MS04]. lutetium [AB00]. iyase [PMM05, CJPS08].
lying [FDSA00, LB08, PRSMV08, ZL05, ZL07, ZL09b, dSVA+09]. LYP
Lysine [DJT08], lysozyme [HN02].
mean
field [KRM+02]. meaningful [AE06, Bud07]. means [Bac05, Bie04b, BLF02, Kar06, KBL08, SMadV00, WKYU01, DOMSL01]. measure [XSHC06, ZHH09, PDC+08]. measurement [YZ04]. measurements [KBLP09]. measures [BDW00, DW08, Ham07, Leh06, PYEA03, PCA+08, PDC+08]. mechanical [AVB00, BISS02, CLP09, CGBF05, CCK01, COL+06, DWC+03, ECA06, ESM06, EBD+01, FHRR07, FGA01a, FAB+00, FAD01b, GAILV01, GLRL00, JHYH08, KMB07, KML08, MLA00, SMDV00, SMAdV00, ZLLS04b, ZLLS05, ZLLS06b, ZKZ07]. mechanical/molecular [CGBF05, FAD01b, JHYH08, KMB07, KML08, MLA00, SMDV00, SMAdV00, ZLLS04b, ZLLS05, ZLLS06b, ZKZ07]. mechanics [AS06, AS09, AD00, AM06b, AGO+02, APG05, BDW00, CLFA07, CR02, CSU05, DPT03, DWC+03, EC06, FEVM01, GCD+08, GS04, GKT05, HWTL03, JCHS07, KLB03, KZRO03, LL00, LLA01a, LL01, LLA01c, LLA03, LSWM00, MLA00, MF04, MPF00, OS03, PRK05, PS09b, PW08, PW08, RMP01, RSE07, RP02, ROG00, RM00, RGP+07, SS00, SHD+08, TGGP+00, TZFRG01, TT05, VSW+00, YSA+03, ZSK07]. mechanics-based [BDW00, RSE07]. mechanics/molecular [MPF00]. Mechanism [CJK+02, LWY+09, PRF04a, Rao00a, AM07, AGK03, BTP09, BLO+02, BS03, CGB+09, CBS+03, DBS07, HP04, HLB09, MLJZL07, JDWS06, JHYH08, KMB07, KML08, MLA00, SMDV00, SMAdV00, ZLLS04b, ZLLS05, ZLLS06b, ZKZ07, ZGZX07, GAVT03]. mechanism-based [PFR04a]. mechanisms [AGI+00, AGI+07, BS06, CCC09, CG05, ILKR09, KZY09, KJJH08, LKLC06, MK02, NS08, RC04, Se01, TB02]. Mechanistic [BMTFR08, SG03, TTD02, Ano06a, ST06, WDS06, XDS06a, ZLLS06a]. media [HLLN06, MM02, SMK00]. mediated [IA03]. medium [FZL+06, HXL09, LF04, LFZS04, SH07, ZFL+05]. medium-resolution [HXL09]. medium-sized [SH07]. melatonin [KKT+08]. mellitus [PS09a]. Melting [LML+00, KT02]. membered [FJ08, ZW09]. membrane [ALB09, CDDK09, DAK08, FCP+04a, GAS04, ILKR09, JM07b, LPB03, MJHS06]. membranes [Ike04, SSM08, WC09]. memoriam [Ano00]. memories [WHRG08]. memory [TYO+02]. mercaptocarboxamides [TFZRG01]. mercaptocarboxylate [APG05]. mercaptopyridine [XYZ+04]. mercury [FNP+06]. Merging [PJPdPRMI07]. Merz [JVK09]. Merz-Kollman-Singh [JVK09]. mesh [BYQS03, KM00, KSY+00]. mesoscope [RPM03, ZBS03]. Mesoscopic [YPNE09]. Met-enkephalin [ZCL09]. meta [DDBP09, ION07, ZTP+08, Gao09]. meta-di-fluorobenzene [ZTP+08]. meta-generalized [ION07]. metabolites [PCMG09]. metabolizing [VB09].
metabotropic [FTLV01]. metadynamics [BBP09]. Metal
[SGD06, ABYM08, Ano06a, Bac05, BTP09, BS06, BRV+07, BM00, BWI+02, CM09, CXZ+09, CWWS07, DSB+02, Dra00, FO08, FKRE08, GM01, GS04, HZX04, Ho05, HSWW00, IC08, JHMB+09, JHMB+11, JKL08, KT08, KRM+02, KEM08, LW07, LML+00, LWK08, LMR06, LS02, LWZ09, MSBS01, NR04, PYCD03, PLC08, RRFC03, SL09, SZT08, ST06, TAS07, VHRR07b, WB07, WWT08, Wa06, YTH01, ZSC05, ZYW+09, ZX08]. metal-catalyzed [HSWW00]. metal-free [CM09]. metal-organic [TAS07].
metal-porphyrins [LS02]. metal-rich [LWK08]. metalic [ALC08, KWK+01, KWK+02, SK08, WLX+05, dVB01]. metalloc [AGO+02, APG05]. metalloenzymes [Sie01]. metalloenzyme [BSDM04]. metallofullerenes [KSN01]. metallofullerenes [CTFC08, KJP+07]. metallofullerenes [KSN01]. metalloproteins [CR09b, SN06]. metals [BP03, BG01b, CM09, LD05a, LK03, LWX+05]. metathesis [PHKG07]. Methane [RRS06, CLC09, EL06, EL07, EM03a, HLLN06, HYR06, IME02, PV07, TMBM02, YQQH09]. methanediamines [CPJ01]. methanol [CC01, YLg06, ZHZ08, ZWP08]. methionine [BP03, BGJ01b, CM09, LD05a, LK03, LWX+05]. method [KFB05, MO01, YGGZ06, ZHZ08, ZWP08]. method-based [KIM+09]. methodological [FDSA00, MFR07]. Methodology [KS02a, SPL+02]. Methods [LSAS01, SB01, AJ03, AGMPRG+08, BB05, BL05, CMaGL+04, CG05, DLD+02, DB07, DM03, DBM03, DDBP09, FOL+04, FO08, GHLK+02, GH07, CY08, GD09, GPN01, GLLR00, GHBB04, HHTK08, IB04, JFG04, KK08b, KBL08, KLE02, KLE03, KB09, LM07, LMB08, LS03, LWH06, LHP01, LK03, LK04, LZF+09, MN02, MZ05, MBWP03, MHT01, MC06, OFB08, PDC+08, PSMB05, Qua04, RSKB03, RCJ02b, RK04, SAM06,
GKTS04, GGT08, GWS+02, HB09, HPL03, HS01, HK08c, HK08d, HHP04, ILB03, JBJB00, JJB02, JPF+00, JBGK08, KSB+02, KFZ03, Lab08, LRI+02, LAR+03, LFZS04, LJ04, LSHR04, LR06, LK03, LK04, LKA01, MWL+08, MPPK01, MCF05, MBC08, Nak07, NL07, OKE+02, PCO+07b, PCO+07a, PMB04, PFC03, Poon01, RMP01, Sen06, TJE03, TCT03, TGGP+00, Tot04, TT02, VW00, VW04, VGDSU08, VP09, WCK00, WKYU01.

model [WS05b, WEE01, WOC+03, WJX+08, XL02, XLT07, YL09, YPNE09, YJF06, vDSSvA04, FCP+04b]. modeled [PB05, vDSSvA04]. Modeling [ECM+03, FRS05, MCR08, Mck07a, Mck07b, MTB09, PSCD+09, SEKS09, Sie01, BA03, BA04a, BZP09, BM08, BSH07, CLP09, CJPZS08, DJT08, DNN05, EDAJ04, ENM+04, GL04a, Gor01, HBM06, HMSM06, HMMS09, HRBKB03, HP04, Hin00, JTO05, KCL06, KSO04, KJP+07, KVS+06, KPZK06, LK07, LLL+08, LFR+04, MML05, MBM+00, MF00, OFB08, SPGS08, SGS03, SY+03, SS05, SPF+07, Sto05, TTB09, VBGL00, XLC08, YKK09, ZBS03, ZMH+09, BBC+05]. modelling [PSHP08]. Models [JB04, AS09, AHGK09, ACM+06, CCK01, CUPGD09, CRG07, CA04, CA07a, CCT+03, DMN03, DLG00, DR07, DDVD09, EC06, FWH+07, FK07b, GSB09, GDV03, GS02, GDPCP+07, GDP08, GS08, HDms05, HDs06, HD06, HP01, HLT+05, HG08, HJCP01, JPF+00, KS02a, Kr03, LJJL08, Lenc06, LS08b, LDTS07, MA05, MCM06, OGH05, OYH05, PJF+03, PA05, QS01, RD06, RSP03, RSER09, RS08, RR05, SBLK01, Sch00, SS+09, SRB02, SKK+07, SB01, SL06, VBS09, WB04a, WB04b, WB05, WZXY07, YCMB00, YGL06, YJF06, YKK09, ZLJS03, ZCL09, ZGFL01, ZLD09, ZWP08, TDH06]. Modern [PB02, FLK+07, Pra01]. modes [Gra07, LSY02, MGLL03, OR05, Tor02]. Modification [HN08, Vya01, WYH04, CM09, FKE03]. 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 [LB08]. Moldyn [RMH03]. Molecular [AS09, BBG+04, BG07, BDW00, CLC09, CLF07, CCK01, DJT08, EMP07, FEVM01, FNP+05, GJK00, HLB09, Ish03, JTO05, KSB09, KAS+07, KLB03, KIM+09, LLA01a, LLA0b, LLA01c, LLA01d, LLA03, LSWB00, MLA00, Maz01, MO09, MS00, MST+08, NB04, Pm01, RMP01, RRZA08, SHD+08, SMD02, VSW+03, WEE01, YSA+03, YGL06, YKK09, ZCZ03, ZWS+09, AM09, ARL01, AS06, AG00, ALB09, AD00, AGMPR+08, ATM03, AM06b, AB09, AGO+02, AP05, AS00, BG03, BP00, BR07, BA08, BB05, BWE05, BRDC02, BWZ08, BVW04, BT00, BS05, BME05, BSJ01, BPCD07, CMJ08, CC07, CDS09, CCL06, COS01, CW02, CI05, CDD+02, CF08, CCSJ00, CGBF05, CF06, CF04, CPC+00, CR02, CCP04, CEP07, CMD+04, CS05, CBH+03, DvG00, DB07, DFT03, DFH05, DFGB09, DPDG05]. molecular [DS03, DCM05, DLHC06, DK01, DWC+03, ESM06, EKB02a, EKB02b, FSM09, FHR07, FG02, FOK+04, FKL+06, FI+07, F01a, FBGO06, FLOD07, FAB+00, FKZ09, FEV+09, FKRE08, FNP+06, FRL09,
molecular [KKS04, LFK05, LL00, LSG06, LFSB03a, LFSB03b, LCKL05, LPK07, LJ04, LTF07, LS05a, LKT04, LM03, LPB03, LEV09, MB00, MFB04, MN02, MBP09, MM03, MABM09, Mas01a, Mas01b, MDA08, MVL05, MH08b, MG00, MCM04, MS01, MPF00, NK01, NYK09, OBS05, OS06, OO04, OO06, OSHS03, OR05, OCP02, ON07, OO08, PMGL03, PRKP05, PMB04, PS09b, PBW05, Pin03, PWHF03, PWHF04, PDS01, Pog06, Ptc01, PRT07, PRT08, PZS04, PYS08, PHH08, PB02, P0208, QTdG08, QNF09, R07a, R000b, RP02, RLE01, RLR04a, RL0109, RSN02, RMHK03, RO00, RGP07, RHL09, S07, SO07, SDL09, SH09, SB08, SE00, SBG09, SY09, STH02, Ste04, SPF07, SVT09, T05, TLK00, TT08, TF04, TGGP00, TZG01, TCR02, TT01, TT05, TR02, TBGR04, UTH03].

molecular-dynamics [WD08].

molecular-loop [PRT07, PRT08].

molecule [ALKH04, BAL01, CLP09, FM00, KK08c, MZ05, NK06, Oos09, Pin03, RG08, SM08b, SFC04, SSW07, SVV08, WLPF05, WDS06, XDS06b, ZZLS06a].

molecule-based [KK08c].

Molecules [LLS02, BG03, BHTCG07, BG00, BZ09, BT00, BKS02, CLP05, CG03, Che01, CR03, CL03, Cul08, DDKV07, DHF05, DR09, DRAS04, EII07, EKO01, FCW06, F01a, FS02, FSO4, GCDL05, GCD04, GB00, HIM07, HDF07, IS07, IC08, JVV09, K030, KGN07, KH01, KP05, KKG09, KGH04, KCH08, KOFF09, Ko04, KvGH01, Le06, LZA02, LYS08, MLS08, Mat03, MSH06b, MS04, MA09, MH08b, MBH02, NMR02, PO03, Pan07, PHJ08, PBS01, PPS08, PSS04, PSM05, RL04, RLR04a, RLR04b, RRZ08, RZWS07, SD09, SH07, TLOG00, TD06, Tor02, VPK08, Van02a, VM07, WCK00, WL04, W01b, WR07, WFR08, Wou00, Y03, YGZ05, YK08, Yos02, ZY07, vEMK01, vE01, vGGB00, PFB05].

MOLEDFIR [PVdJB00].

Moller [CPML08a, DSR07, F1107, Gri03, IN08, JSH07, Var09, WCF02, Y09].

MOLMAP [HMMS09].

MOLPRO [VW03].

molybdenum [BGC09, SS05].

moment [HK08a, HK08b, HK08c].

moments [DVP02, GdSuM07, MLA00, Mar03, PP08b, RP07c, VC04, Y0B08].
momentum \[GY08, WMRW^{+01}\]. mono
\[CU01, GWL07, MMGM07b, HT05\]. mono- \[CU01\]. monoanion \[Bac09\].
monochloride \[ZL05\]. monocopper \[GTC06\]. monoderivatives \[EB04\].
monofluoride \[LB08\]. monohalides \[CWW07\]. monohydrates \[GGP09\].
monomer \[YXC^{+07}, ZM06\]. mononitriles \[Wu06\]. mononuclear
\[CZ05, GK09\]. monooxygenase \[HLLN06, HR06, TMBM02\].
monophosphate \[MRS^{+07}\]. monophosphide \[ZKZ^{+07}\]. monopole
\[ZFL^{+05}\]. monoproteinated \[HA04\]. monosaccharides \[GGK^{+08}\].
monosilicide \[HXD08\]. Monosilicon \[YDWS06\].
Monosilicon-substituted \[YDWS06\]. monosubstituted
\[YDWS06\]. montmorillonite \[DJT08\]. MoO\[LZZC09\].
MOPED \[SRCD03\]. MORPHY \[MP03b\]. Morse \[SDCG02\]. Mössbauer \[HLLN06\]. most \[KAS^{+07}\]. motif
\[HHW^{+03}, LLL07\]. Motifs \[HWT03, WHH^{+06}\]. motion
\[BRDC02, CCSJ00, LPK07\]. motions \[HSWN01, KS05b, LV08\]. Mott
\[RDM^{+08}\]. MOVB \[MG00\]. move \[SM08b\]. moving \[CvG08\]. MP2
\[WD04, BP02, EA08, GCCVB00, IPN06, JPF^{+00}, ME06, PPC^{+03}, SAM06, WD04\]. MP2/cc
\[WD04\]. MP2/cc-pVTZ//MP2/6-31G** \[WD04\]. MpProp \[SKK^{+07}\]. MPSim
\[CWW07\]. MRCl \[KTM02, SWZ^{+05}\]. MSINDO
\[BGJ01b, JGH00, NJ04, SBG09b\]. MST
\[COL01, CSB^{+03}, FBL008, MBH^{+02}\]. MST-based \[MBH^{+02}\]. Mulliken
\[GHBB04\]. multi \[ABWT09, SL09\]. multi-region \[ABWT09\]. multi/heavy
\[SL09\]. multiatom \[SSB^{+03}\]. Multibaric \[OO06\]. multibody \[CPC^{+00}\].
Multicanonical \[HHHS01, SKGS00, YCBM00, KH01, YA^{+02}\].
multicenter \[DBS08, MS01\]. multicentered \[DWN07, HT03, WBSR03\].
multicomponent \[ST04\]. multiconfiguration \[NUH02\].
multiconfigurational \[GD06, JPFJdPRM07\]. multicore \[KHF^{+09}\].
Multicut \[LSHR04\]. Multicut-HDMR \[LSHR04\]. Multidimensional
\[AL01, ARL01, Ch07, HP05, FC00, FC03, RNG03\]. Multidimensionality
\[FVB08\]. multiensemble \[HKMS01\]. multiexponential \[GC03\].
multifarious \[Sim07\]. multifield \[BRDC02\]. multigrid \[BB05\].
Multiisotopic \[Got01\]. multilayer \[LJZ^{+07}, SJJ^{+04}\]. multilayered
\[MR04\]. multilevel \[BHW00, HB00, HBW01, JNY08\]. multiobjective
\[CMBC08\]. Multiple
\[CLF^{+09}, CLZ09, DHW^{+08}, JW06, SK09, ST02, BYQS03, CV09, G09,
KM00, KH06, LJJ^{+06}, MST^{+08}, PAT^{+09}, STCJ08, XOW^{+00}, PYCD03\].
multiplications \[SSB^{+03}\]. multiply \[HT03\]. multipoint \[WS05b\].
multipolar \[DWN01\]. multipole
\[Ami00, ATMK03, BH03, CRG01, CO08, KM00, KLM^{+09}, Mar03, RP07c,
multipole-based [WL09a]. multipoles [KS01a, SKK07].
multipopulation [HHJ03]. Multireference
[WNH03, CWY09, DLD02, HELM09, KBT03, MLL06, ME06, QTdG08, UKNS01, UKN04, WCFH02, dV09]. multireference-MP2 [ME06].
Multiscale [San01, OFB08]. multiscaling [VTT08]. Multispecies
[GDPP08]. Multireference [WNH03, CWY09, DLD02, HELM09, KBT03, MLL06, ME06, QTdG08, UKNS01, UKN04, WCFH02, dV09]. multireference-MP2 [ME06].
Multiscale [San01, OFB08]. multiscaling [VTT08]. Multispecies
[GDPP08]. Multireference [WNH03, CWY09, DLD02, HELM09, KBT03, MLL06, ME06, QTdG08, UKNS01, UKN04, WCFH02, dV09]. multireference-MP2 [ME06].
Multiscale [San01, OFB08]. multiscaling [VTT08]. Multispecies
[GDPP08]. Multireference [WNH03, CWY09, DLD02, HELM09, KBT03, MLL06, ME06, QTdG08, UKNS01, UKN04, WCFH02, dV09]. multireference-MP2 [ME06].
Multiscale [San01, OFB08]. multiscaling [VTT08]. Multispecies
[GDPP08]. Multireference [WNH03, CWY09, DLD02, HELM09, KBT03, MLL06, ME06, QTdG08, UKNS01, UKN04, WCFH02, dV09]. multireference-MP2 [ME06].
Neutral [DWS+09, ASS+02, Bac09, CYM02, DLR+08, EBDPM00, FCP+05, MT03, OSA06, PGG06, ROG00, VM02, Wan09]. neutrals [LLXS02].

neutron [BACJCT01, RMHK03]. nevirapine [AJNG01]. new-generation [YJF06]. Newly [CRS05]. News [Ano04b, BACJCT01, DvL01, Gly06, JVVK09]. Newton [Har04, Qua07].

NF [FJ08]. NH [DMN05, LF02, dOMSL01, DRAS04, ITS05, JPF+00, KT08, KSTC01, LDHR01, MR02, Mck07b, PC00, SEKS09, dOMSL01]. NHC [ZZL+08]. NH NH [LWY+09]. Ni [Bac09, KGL07, PMM06]. NiAt [ZL07]. niches [TP01a]. nickel [Bac09, GKI09, LMIF06, YQQH09]. nicotine [VB09].

nicotinic [GCD+08, SBG+09a]. NiH [ZL07]. NiO [SBG09b]. niobium [Tie09]. NiSOD [PMM06]. nitrate [CGB+09]. nitrenium [FG03]. nitric [JDWS06, LPP06]. nitride [UNM+01]. nitrides [LX07]. nitrido [Bac05].

nitriles [POJ01]. nitrite [DBS07]. nitro [MA05, POJ01, UTH+03]. nitroethane [GWM08]. nitrogen [BGC+09, LLM09, gThDjL+01, WC08, XWL+09, ZLSS04a, ZLSS05, ZYW+09, ZMH+09]. nitrogen-containing [LLM09]. nitrogen-pivot [ZWY+09]. nitrogen-vacancy [ZMH+09].

nitrogenase [Ano06a, Mck07b, ST06]. nitrogenous [Ano06a, Mck07b, ST06]. Nobelium [HdMdS05]. noble [SRB06]. nodal [HYT05]. nodes [Kau07]. NOE [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, JCHS07, SP05, SMV+09, TH02]. noncovalently [PHFC04]. nonelectrostatic [KF02b]. Nonempirical [KSK00]. nonequilibrium [FZL+06, GG09, KK08c, LF04, LFZS04, OD09, YZ04, ZFL+05]. nonhybrid [DF04]. nonsimilar [CRGN07]. Nonlinear [RLA01, BF04, BF07, Har04, HLSH05, MPP+07, WCL05]. nonlinearity [LPK07]. nonmetallic [ALC08]. nonnative [yChHmY08]. nonnucleoside [AJNG01]. nonorthogonal [SMZW05]. nonparametric [HDF+07].

nonplanar [Din00]. nonplanarity [RKH03]. nonpolar [GZL02]. nonrelativistic [WL02]. Nonspecific [LPB03, RGG08]. nonstable [GDPCPU07]. Nonuniform [SHSF05, Bie04a]. norbornadiene [WXK08]. norm [RRS09]. normal [EBAN07, Ksu03, OR05]. nose [BBG+04, QNF09]. Note [Ano04b, Ano04a, FBS09]. Notes [CDGS09, CDS09]. Novel [ILKR09, JHOF03, NL08, TRS02, WL09b, YWHZ03, CRK08, CMBC08, GZL02, GDV03, LXW+09, RIO8, TYO+02, YJF06, ZNNL07, ZL09a]. novo
[LEK07, VGO+07]. Np [Han01, GZL02, Ike04, GHLK+02]. NPAT [Ike04].
NPT [Ike04]. NQR [MH08a]. NR [CPJ00]. ns [CMD+04, SO07]. NSAIDs
[CMBC08]. Nt [ZNLL07]. nuclear [CR09a, CDL06, GM04, HWFN01,
IKN08, QCK01, QCK02, WZXY07, ZPL07, ZXY08]. nuclearity
[BACJCT01]. nucleation [CKW09]. nuclei [CDPL09].
nucleic [CCK01, DP03, DP04, FZL07, FM00, HWTL03, JCL05, MB00, Nak07,
OMNH08, PPYS08, RKKH03, SYC03, SL04, SWR06, SHK+05]. nucleobases
[FKS+09, SB08]. nucleophilic [BSB05, SSB07]. nucleoside [Wil01b].
nucleosides [SA07]. nucleosome [VTT+08]. nucleotide [Mak08, MSF+08].
nucleotides [XWXC08]. nucleus [FVB08, HDsD05, HDs06, HD06, IK08].
NUCS [SHSF05]. nudged [AJ03]. number [CDS09, HXD08, KZRO03, KZW+05,
KH06, TGGP+00, WWL+09]. numbered [GYCZ04]. numbers [GYCZ04].
numerical [DLW06, HXD08, KZRO03, KZW+05, KH06, TGGP+00, WWL+09].
numerical [GYCZ04]. numerical [DLW06, HXD08, KZRO03, KZW+05, KH06,
TGGP+00, WWL+09]. numerical [GYCZ04]. Numerov [Bie04a, Bie04b].
Numerov-type [Bie04a].

O [BL00, GCCVB00, GPSP06, HYR06, ITS06, mJLzY-L+08, KGL07, LZZC09,
LMO09, Mas01a, Mas01b, NA06, Owe05, PGNG03, PGRRM03, UCT+03,
WXCO8, YHD+06, ZJ+07, ZY01, ZZZ04, ZXY03, Bac09, CCJ09, DRAS05,
Dib05, HM08, HD0+02, IS03, LC07, LW04a, LS05b, MGLL03, NyHN06,
NHN06, RAGL09a, RFSS06, SSS02, SRE08, Wil01b, YTY07, ZX09, KZY09].
O-methylation [HM08]. O3LYP [BP03]. OB [NA06]. object [CRH+07, FL08,
MVL+05]. object-oriented [CRH+07, MVL+05]. objectives [STCJ08]. objects
[RSN+02]. observables [MG06]. observations [FWH+07]. observed
[VBS09]. obtain [BVW04]. obtained
[HFS03, VC04, WMW03, WMW04, WHH+06]. obtaining
[Bac04, YGZZ05, SK09]. occupied [HHWG08]. occurring [CJW+09]. OCF
[UTM+02, UTT+04]. OCHF [YLW+08]. OCI [HLLS05]. OCLO [WLZ+07].
OCO [VM07]. OCS [VS02, ZGX06]. octahedral [OSA06]. octan
[BE07]. octan-1-yl]oxy [BE07]. octanol [COL01, CSB+03, Gol09, Tot04].
octanol/water [CSB+03, Tot04]. octet [GR07]. Odd [CC07, GYCS04].
odd-numbered [GYCZ04]. off [HP01, LJKL08, XLT07]. off-lattice
[HP01, LJKL08]. off-plane [XLT07]. OH
[Dib05, Gog08, HTN03, IVSV06, LW4a, Mas01b, WLL07a, CUO1, CUSS03,
GAIVM01, GCCVB00, GGGLL05, HTN03, KZY09, Kle03, KBLP09, LC07,
LWY+09, Mas01a, MGLL03, Mui05, RAGL09a, RAGL09b, SEK09,
UCT+03, WLLS04, WLL+07b, WyLG+09, YLW+08, YLWL09, ZZZ+08].
OH-initiated [RAGL09b]. OH-rotamer [KBLP09]. OH-stretch [Kle03].
OH/Cl [YLW+08]. OHO [Wil01a]. OHS [JP09]. olefin
[PHKG07, YXC+07]. olefins [AVB00]. oligomeric [EL07]. oligomers
[BSG07, CSJ01, Der09, LFR07, SBB02, WCL05, ZOJ+06]. oligopeptides
[MGJAARC00]. Oligovalent [KS02b]. OLYP [BP03]. on-the-fly
On-the-path [CY09, CY13]. One [CR09a, BG03, Bac07, Bie04a, GKRG08, KFD06, Kri09a, Lai07, LB05, ZWS+02]. one- [Lai07].

one-dimensional [Bie04a]. One-electron [CR09a, BG03, Bac07, GKRG08, KFD06, Kri09a, LB05]. one-step [Oos09].

ONIOM [BGCG09, MDA08, MC06, VMF+03, XKKL03]. ONIOM-molecular [MDA08]. ONO [FJ08]. onto [NK06]. OOPSE [MVL+05]. open [CSV+07, FS02, PRSMM03, LLA01a]. Open-chain [LLA01a].

one-dimensional [Bie04a]. Onsager [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 [KB02, KOML08, KDSV02, MT03, POJ01, PB05, XLT07]. OPLS-AA [KOML08]. OPLS-AA/L [KOML08].

Oppenheimer [ZWW09]. opposite [JSHG07]. opsin [RG02]. optical [Bou01, CZFH07, CTFC08, Hua09a, KSB09, LC09, LFR07, MA09, SN06, TDK07, WCL05, YFR05, Zer08, ZX08]. optics [MMP+07]. Optimal [GFS05, ACD+03, BSN06, Blo04, CRG01, DDVD09, SPT07, TTBM09].

optimal-parameter [CRG01]. Optimization [Ano06c, GL04b, GKH05, IK00, WCS09, WM12, AJ03, AM06a, BP00, BdPRMAI00, BM00, Bud07, BLMS08, CS02, CZB07, COS01, CYM02, CLH+07, CY09, CY13, CHMI05, CMB08, DMN03, DV02, FM00, FRL09, GP00, HHH00, HLT0P9, KKA+09, KBA+04, KHF+09, KDG+09, KBL08, KIFK07, LKT04, Mas01a, Mas01b, MG00, MY08b, NYK+09, OS06, OO08, PU09, SRE08, SSMW09, TBGRJ04, UHHN09, VM00, WPH+07, vLBBR12, vVGDM00]. orbital-correlation [SRE08]. Orbital-orthogonality [Pen06].

orbital-valence [MG00]. orbitals [ABF+03, BAC07, BME05, CVVB04, EdlVR+03, FMSA06, GFS05, GC02, HYT05, IN+05, Ish03, JHPRSM+05, Kau07, Kni00, LW07, MS01]. order [Bie04a, DSR+07, FSO4, Gri03, IN08, JSHG07, KGN07, LAR+03, LS08c, May07, MO09, QTdG+08, Rud05a, Rud05b, Rud05c, YH09]. ordering [SM08a]. organic [ATH+03, BLT+06, BT00, CCK01, DA01, EDAJ04, EBD+01, GOL09, HELM09, HP04, JHVF03, JVRK09, JTR05, KLH+04, LH02, LJZ+07, LMRVFH+09, PO03, PB04, SJ+04, SY+03, TAS07, Van02a, WCK00, YGZZ05].

organizing [BA08, ZA07]. organocatalytic [WSM+09]. organocopper
organocuprate [YIN03]. organometallic
[Go01, SY+03, TD08, TTBM09]. orientation [BL00, MWL+08]. oriented
[CRH+07, FL08, MVL+05, RMHK03]. Origin [JS07b, GYMN07, KMM07].
Orthogonal [Bac07]. orthogonality [Pen06]. orthogonalized [Lai07].
orthonormality [ABF+03]. oscillation [CAG07]. oscillations
[DF06, SMK00]. oscillator [AB08, LLM+09]. other [PS03, VMF+03].
oriented [CRH+07, FL08, MVL+05, RMHK03]. Orientation [JS07b, GYMN07, KMM07].
overdetermined [RI07]. overlap [LKW04, SGPS09]. overview
[Sch03, Mac04]. oxazolidones [OY01]. oxazoline [XKG+05]. oxidase
[BS06, JKL08, WZY+04]. oxidases [PS03]. oxidation
[BTP09, DRA05, GCCVB00, GGG05, LB05, RAGLL09b, SS05, XPW09].
Oxidative [DGD+05, LL00, PMM06]. oxide [BSJ01, CFS+08, CCC09, JDWS06, JT08, LPP06, PV07, RRS06, SBB02, ZCS04].
oxide/electrolyte [ZCS04]. oxidized [CNN07, CR02].
oxidoreductases [CFS+09]. oxidosqualene [SGS03]. oxo [CN05, WJX+08].
oxo-porphyrins [CN05]. oxocarbenium [LSB00]. oxoguanine
[FNP+05, JM07a, Pm03]. oxohydrocarbons [Wil01a]. oxoimidazoles
[JKM08]. oxonols [BG00]. oxygen
[GTC06, GW+00, MML+06, SPO9, WSC09, XPW09]. oxygen-adsorbed
[XPW09]. oxyl [AZM03]. oxyl- [AZM03]. oxynitriles [WD08]. ozone
[YLZ08].

P [BAL+01, Gog08, KZY09, LS08a, Lip00, OS08, QB05, WZZ+09, ZY01, MK02, CCP04, Mt01, RPN07, RF06, Tot04, KZY09]. P450
[AST06, HBM06, LCC09, ZAT07]. P450-catalyzed [AST06]. P450nor
[LPP06]. P450s [OYH05]. p8 [BRDC02]. P.Anhar [GBDP05]. package
[AGSFA+05, BACJCT01, CSV+07, GSDT09, IM06, KSY+00, Kh01, KKW+00, MABM09, OTL08, PVdJB00, RMHK03]. package-independent
[OTL08]. packed [AT02]. Packing [MM03, CM09, CA07b]. Packmol
[MABM09]. PAH [DKN07]. pair [FK07a, FS04, GR07, HZ04, KST01, LBT07, MLL06, MGCA07, Nii09, PC05, RC04, SC01, SYC03, Sim07, PC07]. pairing
[DP04, HWTL03, PC05, PC07]. pairlist [HH04].
pairlist-construction [HH04]. pairs
[BM08, CJDK07, FZL07, KKKM07, PABK03, ZZW09]. pairwise
[A05b, CLZ+09, MTE04, Sha05, VP02, VZM+08]. Palermo [Van08].
palladium [WCW08, WCW09]. palladium-catalyzed
[WCW08, WCW09]. pancreatic [MBC08]. paper [JW12, WM12]. para
[ASDP+06, KC01a, ZX09]. para-didehydropyridine [KC01a].
para-didehydropryridinium [KC01a]. para-hydrogen [ZX09]. paradox
[CDGS09]. Parallel
[BWP07, DOSG06, MBW03, TGGP+00, UIHN09, ASW07, A05b, AGSFA+05, BP02, BW+09, CRG01, GBP05, GS04, GT04, GKP05, HHJ03, HHHS01, IS07, IP06, IP07, KKK05, KOFF09, KVF+07, MVL+05, MGJAARC00, NKIS02, NG04, Sha05, SPT07, TYO+02, TFZ01].
Parallelization [GJK+06, PVdB00, PV03, SZW+05, UKNS01, CCWH02, FOK+04, FCK+08, UKN04, VSK+04, vGGB00]. parallelized [TP01a, VK06]. parallelizing [SO07]. parameter [BLMS08, CRG01, CHMI05, HXLS09, MO09, OVMV04, SHK+05, FM00].

Parameterization

[KB02, PNG08, SMM+08, TCT03, BGJ01b, FH01, JKL08, JGH00, LSWB00, MTE04, PB04, RKH03, TGLL07, VSW+03, WK01, JBJ02, JVVK09]. parameterized [GB04]. parameters [AAP00, AMR04, Ano06c, ATBLS04, BBG+04, BSDM04, BZL05, CYM02, DB06, DDVD09, FAR02, FSFK05, FRS05, HPL03, KFNH08, KOML08, KVL+04, KC01b, MMMY07, MRC03, MLL+08b, MLL08, MC06, OYH05, OMNH08, OBT09, PRK05, RRCA08, SO09, SEKS09, SRC03, SHD+08, SF+09, TT05, TTB01a, VCM01, VIP+06, WZW+06, ZSK07].

Parametrization [PDS01, COL01, SBH02, WS05b]. parametrized [RSP03, TAS07]. paraoxon [ZWS+09]. parent [MDI04, 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, BSC+01, Gol09, KC01b]. partially [SVT09]. particle [Ano05b, BYQS03, CZB07, CY08, KM00, KSY+00, LJJ+07, Sha05, SJJ+04, SH07, SZW+05]. particles [BCIB05, WWL+09]. particularly [BS06]. partition [CCK01, CSB+03, DP03, GLD08, Go09, RM07, TS05]. partitioning [ACD+03, DVP+02, DVR+03, HSM06, RP07a, VC04, WNH03]. path [ABBC01a, ABBC01b, Blo04, Bo01, CY09, GF08, GWM08, JP09, Kli01, Qua01, UCT+03, VGB08, WLPF05, WHG+07, CY13]. paths [FG03]. pathway [LGB+09, WLL01]. pathways [AJ03, JW06, LK04, MAF+07, Qua04, RAGL09, RAGL09b]. Pattern [DGHR02, EKB02a, EKB02b, KEB04, AGMPR+08, HWDB03, gWH01, EKB02a]. patterns [CGG06, Gor01]. Pauli [Ish03]. PB [GC04, WHF08].

PBACD [QSS01]. PBSA [PB06]. PbTiO [ZXYF09]. PC [Ano01b, BMIRBD01, HSMT04, OSH03]. PC-GA-ANN [HSMT04]. PCM [FKL+06, CRB03]. PCs [HS07b]. Pd [DDG+05, GBBH09]. PDDG [RCJ02a, TBGR04]. PDDG/MNDO [RCJ02a, TBGR04]. PDDG/PM3 [RCJ02a, TBGR04]. PDE7 [DD08]. pea [PS03]. penicillin [MK02]. penicillin-binding [MK02]. penicillins [DSS03]. pentacarbonylmanganese [SYS05]. pentanes [BPC01]. PEPCAT [OML+00]. Peptide [PDB+04, DHWM+07, HJCP01, JPF+00, ONHN00, PFF+03, BTP09, BWE05, BSP06a, CLW09, CSJ01, CJW+09, CLA+00, CP09, D+G00, DWN01, GSB09, IGNH03, LHJ+06, LL01, MS03, MHT01, MST+08, OGH05, OKH+02, PHFC04, SDL07, Tt04, WCF04, Wil01b, YZ06, YCBM00, ZALMG03, ZCZ03, WHP02, KVS+06]. peptide/HLA [KVS+06]. peptide/HLA-DQ8 [KVS+06]. Peptides [CPML08b, Van08, Ano06c, BBHD04, BCP04, BAH+02, CP08, DJ04, EA08, HHP04, ILYM09, LKJ+04, LLW02, LXL07, MM00, MC06, OML+00, OSH03].
OYK⁺09, OO08, OM04, PCO⁺07b, PRKP05, PFC03, SJW09, WZW⁺06, YAC⁺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, KPZK06, LL03, RLDI09, VBS09, ZM03, AM06a, BL05, BRV⁺07, BLMS08, CCWH02, DF04, DB06, DGI⁺08, FPMS08, KKW⁺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 [GPN01, PZS04]. permutation [SN00]. perovskite [WD08]. perovskite-type [WD08]. peroxa [BLO⁺02]. peroxidase [HBM06]. peroxidative [MRS09]. peroxides [LLZL09]. peroxyl [Dib05]. peroxynitrite [JM07a]. personal [May07]. perspective [KRLD09, LMGO⁺09, PBF09]. perspectives [Fie02]. perturbation [CWY09, CPML08a, CG05, DRMD03, DSR⁺07, FII⁺07, Gri03, IN08, LKV04, MRS⁺07, NCH02, Oos09, PMGL03, Pog06, QTdG⁺08, RSE07, SWZS04, UTH⁺03, UKNS01, UKN04, Var09, WCFH02, WNH03, 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, JKK⁺00, JJH09, KSB⁺02, KT08, KFNH08, KKH⁺07, LRI⁺02, Lee09, LB05, LLL03, MBF04, Mas01a, Mas01b, MM02, Mor02, POJ01, PV07, wQZLy02, QNF09, RRS06, ROG00, SMEG08, SDvG01, SMKM00, TK08, TDH06, UCT⁺03, UNM⁺01, WD04, XKKL03, XKG⁺05, YQHH09, ZALMG03, ZSK07]. phase-space [QNF09]. phases [ALC08, CLP09, LXP08, SK05, XB08]. PhAST [HHG⁺09]. Phe [VKP⁺08]. Phe-Gly-Phe [VKP⁺08]. Phen [ZWS⁺02]. phenol [LL01]. phenols [HM08]. phenomena [KK08c, RSS09]. phenoxycarboxylic [XKKL03]. phenylalaninamide [HJCP01]. phenylalanine [SMV⁺09]. phenylene [ASDP⁺06]. Philippe [Bi09]. phillipsites [LST08]. phonon [EL09]. phosphatase [AG00, FCP⁺04a, FCP⁺05]. phosphate [LDY⁺08, MBL⁺00, PPM05, PHRR08]. phosphates [WOC⁺03]. phosphatidylcholine [CEP07]. phosphine [HT05, LL00, MGLDS00]. phosphine [FLOD07]. phosphine-containing [FLOD07]. phosphininium [LTF⁺07]. phospho [RGP⁺07]. phosphodiesterase [XLZ08]. phosphodiesterase-5 [XLZ08]. phosphohistidine [KVL⁺04]. phosphoimidazole [KVL⁺04]. phosphole [LFR07]. phospholipid [MCR08, RG08]. phosphomannose [RGP⁺07]. phosphonic [CJK⁺02]. phosphorus [LYK⁺04, LTF⁺07, Mit01].
phosphoryl [ZJM+07]. phosphorylation [HLT+05]. phosphotriesterase [KZRO03, ZWS+09]. phosphotyrosyl [OO08]. photoabsorption [CHRL09]. photoadsorption [ZMH+09]. photocatalysts [HZ09]. photochemical [Ama02b]. Photochemistry [GD06, SRE08]. photodetachment [LMCD09]. photodissociation [JHPRSM+05, LXSF08, WXX03]. photoelectron [VDM06]. photoemission [RDM+08]. photoexcited [SRE08]. photographic [Sha02]. Photoionization [MY08b, MY08a]. photoisomerization [GRO+03]. photosynthesis [Ano06b, CPM03]. photosynthetic [IN01, OON01]. photovoltaic [LMRVFH+09]. phthalocyanine [CM09]. phthalocyanines [LS02]. phycobilisomes [MAF+07]. phycocyanin [MAF+07]. phylogeny [LXZ06, ZLY07]. physical [BRS07, DHW+07, OFB08, OS08, SRCD03]. physically [AE06]. physico [AGMPRG+08, Mat03, SB01]. physico-chemical [AGMPRG+08, Mat03]. physico-chemically [SB01]. physicochemical [CP08, CP09, FTLV01, KLH+04, KEM08]. physics [DB02, SPL+02, WS07]. physics-based [DB02, SPL+02, WS07]. physio [CDD+02]. physiochemical [CP08, CP09, FTLV01, KLH+04, KEM08]. physics [DB02, SPL+02, WS07]. physics-based [DB02, SPL+02, WS07]. physio [CDD+02]. physio-chemical [CDD+02]. piano [FKS+09]. piano-stool [FKS+09]. picture [VBGL+00]. Piero [Ano06b]. pinacol [YTY07]. Piotr [Ano06c]. pivot [ZWY+09]. pK [KKS04, ZCS04]. pKa [CFR06, OS06]. planar [CSB08, MMRVH07, SRS07, SBG09b, Wan09]. Planck [DAK08]. plane [PSS+04, PSMB05, RLDI09, VSK+04, XLT07]. plane-wave [PSS+04, VSK+04]. plane-wave-based [RLDI09]. planewave [YK08]. plaster [HP04]. Plastocyanin [SN06]. platform [Gar09]. platinum [CSB08, SMM+08, WM01]. plausible [CBS+03, SB01]. play [YJF06]. Playstation [LEV+09]. pleated [PGC05]. Plesset [CPML08a, DSR+07, FII+07, Gri03, IN08, JSHG07, Var09, WCFH02, YH09]. plot [KMH02]. plots [CLZ+09, SDL+09, SRE08]. PLP [PMM05]. plus [AGMPRG*08, CG05, IKN08]. PM3 [BM00, BSDM04, DC02, GM01, MSH+06b, RCJ02b, TGLL07, TCT03, TBGRJ04]. PM3-compatible [BSDM04]. PM3/d [TGLL07]. PM5 [LKT04]. PMF [Mue01]. pocket [BS08, MDA08, OYH09]. pocket-specific [BS08]. Point [Est07, BCNs07, Bie04a, CRC+08, DWC+03, GDV03, GGLR00, KGL07, KK08a, KFZ03, MGC07, SRB02, TBSM09, WMS06, ZMH+09]. point-charge [DWC+03, GGLR00, SRB02]. points [BMLV04, BAA07, DLD+02, GMA04, HQ02, MP03b]. Poisson [WB04a, WB05, ABWT09, BHW00, BH03, BF04, BF07, DLG00, DAK08, FOL+04, GP01, GCD+08, GGT08, H605, HBW00, HBW01, KWHH07, LDG02, NYTH09, PZS04, SAT004, Vas02, VM+08, WB04b, ZGFL01]. Polanyi [Nye07]. polar [BAÀ07, CYM02, CPML08a, EB04, FA01a, HLLN06, HSF08, JPF+00, PFC03, ZXY09]. polar-neutral [CYM02]. polarisabilities [ZPL07]. polarizabilities [FROD08, LFK05, LYS08, MLA00, MY08a, SKK+07, Tor02, Whe08]. polarizability [BP01, HK08a, HK08b, Mar03, Mor02, QCK01, QCK02, vGGB00].
Polarizable [CFK08, LLM09, Nak07, Ano06c, AGO+02, APG05, BCIB05, COL+06, DGI+08, FKL+06, GWM+00, GS04, GKTS04, GPK05, HHP04, JZD+09, KSB+02, Kol04, LJ04, MMPK01, MBC08, OR05, PWHF+03, PWHF+04, Pom04, RGP+07, TFZRG01, WZW+06, YGLvG06, FCP+04b], polarization [CGB03, CBH+03, EDW07, GGLR00, GKTS04, HK08a, HK08b, JZD+09, KSB+02, Kol04, LJ04, MMPK01, MBC08, OR05, PWHF+03, Pom04, RGP+07, TFZRG01, WZW+06, YGLvG06, FCP+04b], Poly [EdlVR+03, BSOB05, OBBS05]. Polyacenes [ASDP+06, BSJ01, CHA+07, CFD04, MGMM07b, Qua07, SBB02, ZALMG03]. Polyacetylene [PM02]. Polyacrylates [LZA02]. Polyalkaliones [KBLP09]. Polyatomic [GGB07a, GGB07b, RLER04a]. Polyatomic [TGGP+00]. Polycyclic [Bor03, CA07b, FVB08, MGMM07a, VS08]. Polyenes [MW09]. Polyethylene [BCF+09]. Polyketides [KB02]. Polymer [Mei02, BBG+04, CZA03, DJT08, MM07, RRZA08, YSJ09]. Polymeric [Fau01, JCA+02]. Polymerization [BG07, YXC+07]. Polymers [CFD04, CA04, CA07a, DC02, Der09, Din00, DDBP09, HM01, LAEL01, OKE+02, SHH07, VIP+06, YYW07]. Polymorphism [VVBV02]. Polymeric [Fau01, JCA+02]. Polymerization [BG07, YXC+07]. Polymers [CFD04, CA04, CA07a, DC02, Der09, Din00, DDBP09, HM01, LAEL01, OKE+02, SHH07, VIP+06, YYW07]. Polymorphism [VVBV02]. polynuclear [HYR06, RRFC+03]. Polyoxoanions [LFR+04]. Polyvalent [Cri04]. Polyketides [CPML08a, IB04, KF02a, KF03, Nak02, VP09]. Polyphosphate [MRC03]. Polythiophene [CA07b]. POPC [JM07b]. Pople [Ano04a, EA08]. Population [BLT03, BPCD07, Pul05]. Population-Based [Pul05]. Populations [KBN02]. Porphyrin [SBL05, SBL05]. Porphyrin [NyHN06]. Porphyrins [LS02]. Porphyry [AZM03, CHRL09, LPP06, NyHN06, NHH06]. Porphyrin-fullerene [CHRL09]. Porphyrins [CN05, LS02, LWH06]. Portable [SH07]. positron [PRDS08]. possibility [LMGR05, LB08, TT05]. Possible [HIA03, OCP02, WLL01]. Post [WW03]. post-HF [WW03]. Posteriori [SPDS01]. potassium [MCR08, MHS05]. potential [AMR04, AE06, ABBC01a, ABBC01b, BCS07, BL05, Bob01, BBI+09, DMLI05, DMC05, DLHC06, DK01, FSFK05, FKKRE08, HPP00, HHRKB03, HPL03, HFS03, IS03, IT03, JZD+09, LFK05, LMK01, LS08c, MMLC05, MCF05, Nak07, NG04, NMTA01, PBC+01, Qua01, RD06, RNG03, RHL09, RTG00, SPDS01, SS00, Sch03, SMGE08, SSS+09, SHH07, SG07b, SBB02, SJW09, TBSM09, TLKT00, WCC08, WLD09a, WCK00, WS07, YH06, YHD+06, ZCS04, ZZY07, ZZY08, ZGXX06]. potential-derived [TBSM09]. potentials [ATM+07, CLC09, CU09, CW09, DB02, FAB+00, FNP+06, GK09, GBJ03, HXZ04, HHHS01, HZ06a, IYK09, KHL+04, KCK+08, KK01b, LJ07, LHI09, LK03, LK04, LLW+09, MCF05, MWE02, OR05, PML03, RPMP03, RLER04b, SMDV00, SPT07, VGDSU08, dSR08]. Powder [HWDB03, IHI03, GWH01]. powerful [PSDM00]. pp [Bic09, Lip00, Sta00]. PQS [BWM+09]. PR [AVS09, VVS07]. Practical [BMRDB01, PHR+05, WOO11, You11, Blo04, Sch03, SHSF05, SWZS04].
Precise [Ami00, Ara04]. precision [CN03, GAdGM08]. precursors [CFD03, CFD04, DJT08]. predict [HL08, HZ06a, HZ06b, LL07, PB06, PJPMdPRMI07, XSHC06, XLC08, YMT04]. Predicted [PDP02, IGL07, JARM02, KCL06, WS02b, ZCL09, ZGXX06]. Predicting [DR09, Der00, LKA01, ZLJS03, AG03, CLXC02, CRGN07, IO08, KS02a, XWC09]. Prediction [AVS09, CLC03, CKR08, CJDK07, IO08, KS02a, XWC09]. predictions [BS01, BLB09, CP08, Ruv07, Van02a, ZLD09, vEMK01, vE01]. predictor [Kol04]. prefacess [FA01b]. preferences [GSB09, KK09, LKJ04]. preferred [DV02]. preliminary [KMH02, PM+08]. Preprocessing [SHM04]. prerequisite [WHF08]. presence [LZA02, RAGLL09a]. present [GR07]. Presentation [Rud05a]. preserving [QNF09]. pressure [Car02, MTB09]. pressures [TK08]. primary [HB09, JIK09, KBN02]. primitive [MV06]. principle [GJL08, PRS04, ZDS05]. principles [CS01, EBL08, GD09, HZX04, Hua09b, KK08c, MLJ03, TK08, VP08, WLX05, WZZ09, WD08, ZXYF09, ZHMW09]. prion [IKK09]. priories [SPDS01]. prismatic [WL09a]. probabilistic [PJB07]. probabilities [DP04]. probability [CFS03, DLW06, GCDL05, Kn00, SK09, SCS07]. probe [CVR08, DML05, TH02, VSW03]. Probing [PAT09, WMGK07]. problem [ABB01, ABB01b, An06, Bo01, CCL06, HLLP09, Qua01, ST06, TKH07, XOW00]. problem-size [HLLP09]. Problems [You11, ABWT09, Mat03, Vis02, WLL09]. Procacci [An06b]. procedure [AM09, BR03, CA07a, DLSV00, G06, KBT03, RS08, SSL02, SMM08, YCBM00, Zho06]. procedures [GT03, HSMT04]. process [BZL05, LG09, ML00, Pac06]. processes [Che01, GG09, KEM08, LDT07]. processing [AG100, AG107, FEV09]. processor [LEV09, Yas08]. processors [SPF07]. Producing [KB02]. product [SFR07, YLW08, YLW09]. production [YQQ09]. products [KYFW07, LZ05b]. PROFASI [IM06]. profile [Ber03, CCB04, CCP04, GB02, ONH00, Zho06]. profiles [AHK02, CMBC08, OD09, YXC07]. program [AJ03, BBM09, BAH02, DRMD03, GRC01, GLY06, GM04, IS07, KLI01, KWK00, MP03b, ME06, PPX01, PRJ02, QQ01, RMMH03, SFRS01, SMZW05, TRS02, UHH09, VB07, VPK09, Zer08, BBC05, BK02]. programmable [Gan09]. programming [SPT07]. programs [CC05, KS08, MBP09, SH07]. projection [FS00b, GKH05, GY06, Qua04, TKN08]. projector [MOP07].
projector-augmented [MOP+07]. prokaryotes [WHH+06]. prolapse [HdMdS05, HdS06, HD06, TW03]. proline [BISB02, KK09]. promising [JR01]. promolecular [Leh06]. promolecule [MS00]. promoted [SBG09b]. promotion [KMM07]. propagator [SVT09]. propanal [RR05]. propanone [RR05]. propargyl [LMK01]. propellanes [PAS07]. propenal [FDSA00]. propene [BS03]. properties [AB00, AEE+03, ÁCD+03, Ara04, AZS+04, BG03, BZP09, BT00, BSOB05, BACJCT01, CM08, CDGS09, CDS09, CPDZH08, CLC09, CVR08, CZFH07, CDD+02, CHA+07, CRSB03, CTFC08, CMA+08, DD08, DXW08, DWNB01, DVP+03, DD00, DPM09, DSS03, DHW+07, EM03a, EM03b, Fan01, FTLV01, GKRGO8, Hua09a, HJCP01, JPF+00, JWB05, JTO8, KHY00, KLH+04, KJP+07, KLC00, Kri09a, Kri09b, KGD06, KPZK06, KK01b, LTF+07, LWLS07, LC06, LFR07, LLZL09, LMRFVH+09, MV06, MM02, MA09, NA06, NINAT+07, NAT07, OBBS05, OS08, PM04, PK04, PBF07, PTC01, PSS+04, POJ01, RKA+09, SBJ08, SRK+00, TZX01b, TZX01a, Tor02, TDK07, UM03, VB09, VKCK09, VP08, WLX+05, WM06, WCL05, YFR05, ZY01, ZXYF08, ZW08, ZK07, ZMH+09]. properties-based [VB09]. property [BAA07, JLHF03, NLL+09, PSCD+09]. propylene [QZL+04, RR05]. propynyl [Lee09]. prosthetic [ATBLS04]. protease [BWE05, CLXC02, DLG00, LZ05b, NLL+09, SPT+03, SVV+08, WHF08]. protease-inhibitor [SVV+08]. Protein [LEK07, NCO+05, PJB+07, ADM+06, AG00, AHGK09, BED02, BRDC02, BMLV04, BS01, BSP06b, BS05, BSH07, BLMS08, CCC03, CLXC02, CLC03, CLW09, CLS+09, CIB05, CLH+07, CKR08, CLF+09, CJKD09, yCkHM+08, CRH+07, CPUGD09, CSRST04, DHM+03, DPRR05, DB06, DB02, EBAN07, FOL+04, FC06, FKM+06, FKM+07, GLD08, GHH07, GL04b, GCO4, GDPCPU07, GdSVM+07, GHMP03, GKK07, GZM09, GB04, HEP+02, HFS+07, HP01, HS01, HM06, HLTL09, HLM05, HLTP+05, HZ06a, HZ06b, HG08, HW09, HP05, ILKCR09, IM06, IK09, IT03, JS07a, JMD+02, JIK09, KFB05, KFNH08, KLS02, KLC06, KHF+09, KKO1a, KIFK07, KH05, KFO8, LFBSK07, LHJ+06, LJKL08, LV08, LZKT04, LXW+09, LL07, LW06, MB04, MKT04, MLG04, MHI09, Mi02, MWE02, MLL08a, MHT01, MP00, NMAT01, OFB08, OFK09, PB06, PHR+05, PC00, PFC03]. protein [PSHP08, PMM05, PB02, PF06, PNG08, QLH09, RI08, RSR09, RLP08, RSO8, RK05, Ruw07, SHM04, SLT+09, SWM04, SVV+05, SN06, SR09, SMD09, STC08, SL06, TLKT00, TGD05, VW00, VW04, VGO+07, VGDrots08, VGGMM05, VZM+08, WS05a, WS07, XZ04, XSHC06, XLC08, XWC09, Yan04, YLO6, YFS07, YPNE09, Yos02, ZP03, ZGFL01, ZSO4, ZZ08, ZTS09, ZM06, dSR08, HLC09, PBM04, ZZTS09]. protein-DNA [PSHP08]. protein-environment [HFS+07]. protein-tyrosine [AG00]. protein-tyrosine [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, LHJ+06, LKA01, MK02, MSH+06a, MZL08, NAT07, OS06, OSHS03, OM04, PB04, PMG04, PRJ02, RGZM09, RON02, SL09, SPL+02, SHBD05, SHSF05, SMV+09, VBS09, WZW+06, WM06, WS05b, WHH+06, XZ05. Protocol [AGI+00]. Proton [SRB06, AGK03, BA03, BA04a, CXZ+09, FDSA00, FO08, GWM08, HFHL06, LLM08, LMGO+09, LB05, MA05, PGG06, PCS04, SM06, WFHP01, WHP02, XKGM05, ZCS04, dSGCG00]. proton-coupled [CXZ+09]. protonated [CPDZH08, ZDS+05]. protonation [Bac05, CG05, DHM+03, HP05, KYFW07, WHF08, XZ05]. protoporphyrinogen [WZY04]. prototype [Aug09, CS01, ASDP+06]. prototypes [SSS+09]. proximity [Agr03]. pruning [TCSM03]. pseudo [LL07, VDM06, XSHC06, XLC08]. pseudofolding [VGDSU08]. pseudoknots [DP03, DP04]. Pseudomonas [NYK+09]. Pseudopericyclic [LFS+07]. pseudopotential [FMAMVK06, LK03, VW03, vW06]. pseudopotentials [FSS+04, PSMB05, SMD02]. PSi3 [CSV+07]. psoralen [NBTN04a, NBTN04b]. Pt [DMN05, LK03, RW08, LF02, RD00]. PtCl [LF02]. PtF [LF02]. PtH [LF02]. Pu [Han01]. pump [CR09b]. pump-probe [CR09b]. PUPIL [TdMSD+08]. Pure [MDI04]. PyFrag [VGB08]. pyrazine [LWX07]. pyrazole [DMC05]. pyrazoline [LLKC06]. pyrazolyl [HT05]. pyrene [HIA03]. pyridine [CHA+07, HT05]. pyrimidine [LWX07, XWXC08]. pyridine [CHA+07, HT05]. pyridines [WRP+06]. pyridoxal [LDY+08, P1M05]. pyridyl [LWX07, XWXC08]. pyrimidinyl [WJX+08]. pyrolysis [KKH+07, XKKL03]. pyrolysis [KKH+07, XKKL03]. pyroprobe [ZKZ+08]. pyVib [Zer08].

Q [BS08, KWK+00, WHG+07]. Q-Chem [WHG+07, KWK+00]. Q-Dock [BS08]. QCSID [ZKZ+07]. QCT [DMJ+09]. QM [CGF05, MPF00, AGK03, AST06, AB09, CR09b, CG05, FAR02, FMSA06, FSFK05, GWM08, GWM+00, HHBH00, HBM06, HNR08, HR05, HT03, HTN03, IV04, IvSV06, ITS05, IT05, KHF+09, KBLP09, KPR04, Kri08, Kri09b, LLL03, MBM+00, MK02, MSH+06a, MG00, MLJ03, NGTB03, RG02, SURG06, SBG+09a, SN06, SM3+08, SVV+08, THHN01, TdmSD+08, VFZ+03, WCC08, WHG+07, WC08, ZWZ09]. QM/FE [AGK03]. QM/MM [CGF05, MPF00, AST06, CR09b, CG05, FAR02, FMSA06, FSFK05, GWM08, GWM+00, HHBH00, HBM06, HNR08, HR05, HTN03, IV04, IvSV06, ITS05, IT05, KHF+09, KPR04, Kri08, Kri09b, MBM+00, MSH+06a, MG00, MLJ03, NGTB03, RG02, SBG+09a, SN06, SM3+08, SVV+08, THHN01, TdmSD+08, VFZ+03, WCC08, WHG+07, WC08, ZWZ09]. QM/QM [AB09, HT03, SURG06]. QMCF [PHHR08]. Qmd [KMH02]. Qmd-plot [KMH02]. QMPFF3 [AGI+00]. QMQSAR [DML+05]. QSAR
[DHW+08, DHW+09, SGPS09, CGMPT+08, CMBC08, CRGN07, DMLI05, DMC05, GDPP08, HSMT04, HMM09, LLL+08, LJJ+07, LSY02, MR09, PS09a, SJ+04, TCSM03, VB07, VB09, GDFSU08, XYN+06, ZNLL07].

**QSAR-analysis** [VB07]. **QSAR/QSPR** [TCSM03]. **QSPR** [CDGS09, CDGS09, CDGS09, GS08, HM08, TTRM09, TCSM03, ZNLL07].

**QSPR/QSAR** [ZNLL07]. **QTAIM** [MGMM07b, RKA+09]. **quadrature** [CG06, DBS08, GC03]. **quadrilaterals** [GKK07]. **quadrupolar** [CMA+08].

**quadrupole** [HLLN06, HK08a, HK08b]. **quality** [BG03, CMJ08, EM03b, FKZ09, JBJB00, JJB02, SSS+09, TSSGS07].

**quantifying** [GT03]. **Quantitative** [Mit01, WZY04, YNZ+08, BAA07, CDGS09, CDGS09, DHW+08, DHW+09, Gra07]. **quantization** [GLMV09]. **Quantum** [AVB00, BWM+09, BISB02, BS06, DMN05, ECA06, ESM06, EDA04, FHRRO7, LBT07, MBL+00, MA05, NRKH02, PM02, RM07, RON02, SC01, SS05, TLOG00, VHRR07a, ZMH+09, AGMPRG+08, AGO+02, APG05, ATH+03, AGSFL05, AGSFA+05, BS01, BP070, CLP07, CDGS09, CZFH07, Con02, CKW09, COL+06, DBS07, DBM03, DA01, DWC+03, EBD+01, FCK+08, FA01a, FAB+00, FKFG08, FR06, FUK+05, GAIMVB01, GATG03, Gog08, GBB07, GGLR00, GS04, HM08, HHP04, JJH01, JCHS07, KSB+02, KFNH08, KJVW08, KHY00, KZRO03, KLM+09, LX07, LHP01, MFB04, MP03a, MGCA07, MKTO4, MR09, MBP09, Mat03, MC06, MF00, OYH05, OKH+02, PG04, PHKG07, PDS01, PV07, RP07b, RSE07, RGP+07, SF07, SH07, SS00, Sau04, Sch00, SFRS01, SBB02, TCR+02, TT02, VHRR07b, Vis02, VKCK09, WS05a].

**quantum** [WOC+03, XYN+06, XZZ04, XLZ08, ZC03, ZAT07, ZSK07, SB08, CGBF05, DSS03, KBL08, PFB05, SCS07]. **quantum-chemical** [DA01, SFRS01, VKCK09, XYN+06]. **Quantum-connectivity** [EDA04].

**QUantum-regions** [SB08]. **quartet** [MSB01]. **quartet/metal** [MSB01]. **quartets** [MSB01]. **quartic** [SAS05]. **quartz** [ZWPR+04]. Quasi** [AGI+07, NUH02, AGI+00, ITN+05, VMA03, YH07]. **quasi-canonical** [ITN+05]. **Quasi-degenerate** [NUH02]. **quasi-flexible** [AGI+00]. **quasi-relativistic** [VMA03, YH07]. **Quasirelativistic** [HWFN01].

**quaternary** [CW02, SO07]. **quaternions** [CSD04, CSD05, Kne05]. **Quick** [LMV07]. **QUILD** [SB08]. **quinolines** [KS05c]. **quinoprotein** [JJH01].

**quintet** [GWL07].

R [Bo01, CP00, LZZC09, Lip00, Qua01, ZY01, LZZC09, ZPL07]. **rack** [OCP02]. **Radial** [GC03, ESP04, Kau07, Kni00]. **Radical** [XDS06a, AVB00, BLO6, CUS00, CU01, CUS03, CZX+09, GSB09, HIA03, JDS06, KOML08, KKMM04, LC07, LMK01, NSB08, O004, gThDjL+01, WDWS06, WDS06, WDSZ07, WYG+09, WLL+07, WLL+03, XDS06b, YLW09, ZLLS04a, ZLLS05, ZLLS06a, ZLL+09, CXZ+09, QZZZ03].

**radical-molecule** [ZLLS06a]. **radicals** [BE07, Dib05, Lee09, WLLS04, WDSZ07, WSC09, YLW+08, YLW09, ZM03].
radii [OCB02, PML03], radon [HD06], Raf [GC04], Ramachandran [SDL^09, GSB09, HHP04, PFJ^03], Ramachandran-type [SDL^09], Raman [Bou01, LC09, NKRH02, OBBS05, Zer08], RAMSES [BMRDB01], random [CY09, CY13, CA04, HXL09, JS07a], randomized [LFK00], range [CEP07, GPK05, Gri06, HGB04, IZA06, JPCA08, KSS08, MN02, RP07c, RLP08, San01], range-separated [JPCA08], rank [RP07c], ranked [TBSM09], ranking [KSM05], Rapid [GGAO0, RSN^02, BH03, Gra07, KMH02, WS05a, PABK03], Rapidly [KF02b, Zo06], rare [LZZC09], Ras [GC04], rate [Chu07, GGB07a, GGB07b, JHZ09, MGLL03, NSU^02, SLL^04b, SFRS01, UCT^03, WLL05, WLL^07b, WDX^02, ZP03], rates [HG08, JIK09], Ratio [LR06, KBB09], Rational [Chi03, BSP06a, Ham07, VGGMM05], rationalized [Bac05], rattle [FS98, FS00a], ray [HSWN01, HN02, WKYU01], Rb [GLRL02, GWL07, HRR05], Re [LJKL08], Re-examination [LJKL08], Reaction [CU01, JKM08, JDWS06, KKJ08, MGG06, Qua04, WCHW09, ABBC01a, ABBC01b, BAL^01, Bie04a, Bo01, BS03, CUSS03, CG05, DRAS04, DRAS05, FG03, GZL02, GF08, GWM08, Gog08, HLLS05, Hir08, HLHS05, HTN03, IN01, JH01, JHZ09, LMGO^09, LMK01, LL01, LFZS04, LW04a, LDT^02a, LDT^02b, LWY^09, LLL07, MGLL03, MG00, MS04, Mut05, NSU^02, OON01, PGNG03, PGRRNG03, Pom04, PS03, PM06, wQZsLyZ02, QZL^04, Qua01, Qua07, RSN^+02, RD00, RWHB09, RJLR06, RR05, SLL^+04a, SLL^+04b, SRE08, TYN05, gThDij^01, TGLL07, TMBM02, UCT^+03, VGB08, WLL01, WDWS06, WLL^+07b, WCW08, WHG^+07, XDS06a, YLZ08, YQQH09, ZLL04, ZLLS04a, ZWL^+05, ZLLS05, ZLS06a, ZLS06b, ZZW^+07, ZLL^+08, ZLL^+09, dRLLS00], reaction-diffusion [Bie04a], reactions [AM07, BS03, CUS00, CFD03, Fie02, GAIMVB01, GMA04, GLH^+08, GGB07a, GGB07b, HFHL06, HSWW00, JM07a, mJZsLyL07, mJZlyL^+08, JHZ09, KIMF07, KL00, LDC^+07, MBL^+00, NTH00, OY01, OY03, RNG03, Rao00a, RC04, RY09, Rud05b, Rud05c, Sch03, Sie01, SSB07, TTT08, TCR^+02, UNM^+01, VBGL^+00, WLLS05, WLS06, WLO7a, WyLG^+09, WDX^+02, WLL^+03, XLL^+02, XDS06b, YT04, YLW^+08, YLWL09, ZLLS04b, ZKZ^+07], Reactive [LLM08, Hir08, MMMY07], 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, ZGXX07], rearrangements [LLKC06, YTY07], Reassessment [DBM03], Reassociation [DNWN01], recently [RG08], RECEP [KC01b], receptor [DLRZ09, FKA^+05, FKM^+06, FKM^+07, GCD^+08, HMK02, KBK^+01, MHL^+09, SBG^+09a, TFN04, TJE03, WS02b, XWC09], receptors [CW02, FTIV01, NHH05, YKK09], ReCO [HT05], Recognition [UNHYT06, AGI^+00, AGI^+07, AGMPRG^+08, BR07, CW02, DGHRR02, EKB02a, EKB02b, GdSuM^+07, KEB04, MSF^+08, PSHP08]. 
Reconstructing [BBP09]. reconstruction
[Adc04, GKK07, KLS02, RS08, TGD05, WG02]. recoverin [LGB+09]. red
[McD08, SRK+00]. red- [McD08]. redesign [GLD08]. redistribution
[ZY01]. RedMD [GSDT09]. redox [GK09]. Reduced
[BR04, BSOB05, OBBS05, ABBC01a, ABBC01b, BMLV04, BoI01, CNN07,
CP08, DLD+02, EII07, GSDT09, HP01, Qua01, RS08, WEE01].
Reduced-size [BSOB05, OBBS05]. Reducing [PRSMM02, SSL02, SY09].
reductase [CFER04, CGB+09, CBC+08, DBS07, GGLR00, HLLN06, LPP06,
PCS04, PFR04a, PFR04b, TMBM02]. reduction
[C CCCJ09, DBS07, DMN05, HLTLP09, LRWG03, Mck07b]. reductive
[PS03]. reevaluation [Kle03]. Reference
[ZZ08, CF04, CFC+08, LZ05a, NUH02, OV03]. Refinement
[HB09, Ruv07, BHW00, MM05]. refinements [GPK05]. Refining
[CLWL09, SB01]. refractive [YYW07]. regarding [KZY09]. region
[ABWT09, Ama02a, HHHB00, WEE01]. Regional [TKH03, NTH09].
regions [HYT05, SB08]. regioselectivity [AVB00]. Registering [GBL+05].
regression [DLWV07, GoI09, GS08, LCC09, SY09]. Rehybridization
[AM07]. related [ALC08, ACLD03, CFD04, KC01a, LXW+09, LHW06,
LCDA03, LCGA03, LCA03, ML00]. Relation [SM08a, DVRP+03].
relationship
[DHW+08, DHW+09, JPCA08, KWK+01, WLX+05, KWK+02]. relationships
[BAA07, CDGS09, CDS09, CPUGD09, JLFH03, PSCD+09, WZY04].
Relative [SWV+05, BLB09, CG05, MML+06, MRS+07, RSE07, ZOJ+06].
Relativistic [FHF+01, NYI02, NSO+07, SNM+06, SMD02, WTKM06,
YH09, ASS+02, BB+09, Dya02, GHLK+02, GPSP06, HDMdS05, HDs06,
HD06, LF02, SH02, Van02b, VMA03, WL02, YH07]. relax [GFS05].
relaxation [BRDC02, HS01]. relaxed [AEE+03, CA07a]. relevance
[An06a, MGCAC07, ST06]. reliability [IB04, LKW04]. reliable
[BE06, WHF08]. remove [LZ05a]. removing [PCS04]. reordering
[TVL+03]. reorganization [FZL+06, KMM07]. repair [Pin03].
reparameterization [RFSS06]. repeat [NK01, NL08]. Repeated [KH01].
Repeated-annealing [KH01]. replica [FSM09, FGR07, GLP08, NCO+05].
replica-exchange [FGR07, NCO+05]. Reply
[Bo01, CPML08b, WM12, CSD05]. Representation [GPK05, BB08,
CKR08, CF06, JIK09, LW40b, LXX06, LW06, RLR+04, WEE01, hYD+08].
representations [BMILV04, LAR+03, LR06, RS08, SN00, YNW05].
representative [YLL+09, YXL+09]. reproduce [VBS09, WS05b].
reproducing [MF04]. repulsion [COL+06, Kri09a]. repulsions
[HGMB04, PB09]. repulsive [BDV00, CFC+08]. requirements [AM06b].
research [JLFH03, PGH+04]. residual [RI08]. residue
[MH09, NBTN04b, PPM06, NBTN04a]. residues
[CFS+09, DHW+07, HJCP01, JPF+00, OS06, UNHYT06, XLT07]. resolution
[BS05, BS08, CDGS09, DSR+07, GL04a, HXLS09, Nee03].

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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 [MLVG06]. s-tetrazine [XZ04]. SA [GC04, GWS+02, 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 [LZKT04, BHG03, CN03, CIB05, CY09, CY13, CV09, CvG08, CEPO7, DDVD09, FKZ09, GT03, HKMS01, IS03, JW06, KH01, KM07, LKW04, Mak08, MH08b, MSH+08b, Nak02, NA06, RNG03, Rap06, SD09, SMG09, TS05, YL06, ZA07]. sand [JD09, RPNJ07]. sandwich-like [JD09]. sandwiched [MHS05]. sarcoplasmic [HLB09]. SARS [LZ05b]. SARS-CoV [LZ05b]. SASMIC [EA06]. Sason [Bic09]. Sb [LS08a, XB08, XK08]. Scalable [PBW+05, VSK+04, Ana05b, KKCI05, SHA05, VGO+07]. scalar [GPS+06, KBLP09, MP03b]. scale [DMN03, JO02, KKCI01, MH09, MHW04, MFP00, ME06, Nak02, NA06, RRS07, SSL02, TY0+02, 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, vGGB00, vDGDM00]. scanning [HM02, MFR07, SMGE08, ZM06]. scattering [BACJCT01, Est07, HSWN01, RMHK03, WKYU01]. SCC [ECM+03]. SCC-DFTB [ECM+03]. SCF [JHPRSM+05, PFJ+03, PVJBO00, SAM06, VZVG06]. SCH [ZZW+07]. scheme [Bac04, FOK+04, IS03, JCA+02, JVVK09, LMV07, Maz08, MSH+06b, RKA+09, SR07, WS05b]. schemes [Bac04, Bac05, Bac07, PR04, SPDS01]. Schleyer [Lip00]. SCI [TY03]. SCMP [FA01a]. SCMP-NDDO [FÁ01a]. SeCO [LMCD09]. Scope [LFEdL06]. 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, LZO5b, PRDS08, SHSF05, YOB+08]. SCRF [CCT+03]. SCUD [LZ05a]. SeX [WWS07]. SD [WLLS05]. SDCl [BMB07, PRSM02, PRSM03]. Se [HKHN08, JJK+00, WWS07]. search [AM09, BR07, BMBC01, CSJ01, CA04, GLD08, HHG+09, HXL09, HM06, IZA06, KK01a, LFKL00, MGJARC00, NL08, OGH05, OM04, Pol05, RRHL09, Sau04, SE07, SE08, WKO1, ZA08]. searches [CZB07, YXL+09]. Searching [SPT07, STC+08, CvG08, Nak02, OY09, SCC04, SYC08, YCS07]. Second [BC06, FS04, MO01, AGK03, DSR+07, DOSG06, FO08, IN08, JSHG07, LC04, QTdG+08, QCK01, QCK02, RUD05a, RUD05b, YTH01, YH09]. second- [LK04, Rud05a, Rud05b, Rud05c, YTH01]. Secondary [FS04, DSR+07, IN08, JSHG07, QTdG+08, Rud05c, YH09]. secondary
[CLC03, CLA00, DW08, DP03, GdAcV07, IGNH03, LhWX07, LCSZ09, LW06, LOL08, LLL07, MHT01, WPH07, YNW05]. Section [Ano01c, Ano04b]. sections [MY08b, MY08a]. seedling [PS03]. segment [YS00]. segmented [CGS4ST06], segments [BTLP03, GAS04, KF02a, YMT04]. segregation [Sza08]. Selected [BMB07, LSAS01, Mat03, PRSMM02, ZOJ06]. Selecting [HXLS09]. selection [HW09]. Selective [TCSM03, XPW09, AM06b, MHL09]. selectivity [BSPO6b, GLRL02, O008, ZZvRSC08]. Self [ZA07, BA08, BWI02, ECM03, NUH02, NTH09, NL08, SH07, TKH03, VTT08, WM04, XL02]. self-associative [NL08]. self-consistent [BWI02, NUH02, VTT08, WM04, XL02]. self-contained [SH07]. self-interaction [NTH09, TKH03]. Self-organizing [ZA07, BA08]. semi [BBH04, UKN04, ZNLL07]. semi- [UKN04]. semi-empirical [ZNLL07]. semi-implicit [BBH04]. Semiautomatic [PRJ02], semibullvalenes* [HWGB01]. semiclassical [KM07]. semicore [HZ09]. semidirect [MBWP03]. Semiempirical [Gri06, LKT04, TT01, BUMCMRL00, BM00, Der09, DMLI05, FBLO08, F008, GGLR00, HM0G07, IK00, JFG04, KSS08, KBT03, LMMW04, MAF07, MHT01, Nye07, RSKKB03, RCJ02a, RCJ02b, SBL05, TCR02, TBGRJ04, vdVGD00]. semiempirical-DFT [Der09]. Semiglobal [DV02], semi-microscopic [KK08a]. semirigid [CLP05]. sensitivity [HLSH05], sensitization [Sha02], sensitized [KS05c]. sensors [BBG04]. Separable [EA06], separated [JPCA08, MLL06, WSM09]. separating [CN03], separation [FBGD06]. sequence [AM06b, CCWH02, CKR08, CLZX09, Dya02, JIK09, LXZ06, LSW01], PRJ02, WHH06, ZLY07]. sequence-dependent [LSW01]. sequence-specific [PRJ02], sequences [CP09, DLW06, DLWV07, Der00, JIK09, LW04b, LD05b, LW06, N007, PP08a, hYDN08]. sequential [TT05, ZGZX07]. SER [JPF00], serially [KMA07]. series [CC07, KMH02, PDS01]. serinamide [PFC03]. serine [OBT09]. serotonin [HLC09]. serve [Mck07a], set [ABF03, ALK04, AHK02, BR04, BT00, BSOB05, BRV07, BRLS08, BRLS12, CMJ08, Che01, DMZT08, EL09, EKB02a, FZL07, F008, GGLR00, GGT08, HDML05, HMSM06, IO08, JKK00, LF05, MV06, Mas04, MLL08b, MC06, PSC01, PRK05, Pen06, PFJ03, PSMB05, RRP01, SSB03, SHK05, TW03, VKP08, Var09, VKCK09, WMGK07, Wb04, WG02, ZWPR04]. set-up [GTT08]. sets [BY06, BSOB05, CRS05, Cu04, EA08, EdIRV03, GKH05, HDs06, HD06, IO08, KK08a, LST08, LTV08, MV06, NS09, OBB05, OVMV04, RLA01, RLE01, RLER01, SNM09, 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, MLG03, Mui05, SSS09, WLLS05]. SH/ [SSS09]. SH3 [IGNH03]. Shaik [Bic09]. shake [KFDO6, BL09, FS98, FS00a, KVGH01]. shake-up [KFDO6]. Sham [Bou00, RRS07, SH02]. Shannon [LM03]. shape
shape-based [PRDS08]. Shaplets [PRDS08]. shapes [BR07, KS02a]. sharing [HS07]. sharing [BR07, RS07a, RS07b]. SHARPEN [LMH+09]. Shaw [Ano05b]. sheet [KF03, PP08a]. sheets [LLW02, PG05]. shell [DSB+02, FS02, FO08, HB09, PRSMM03]. shielding [CDL06, CDPL09, HWFN01, MC06, PFC03, WZXY07, ZPL07, ZXY08, ZLD09]. shift [Dra00, HP05, LFZ04, MA05, RG02, WPS02, XZ04, ZFL+05]. shifted [Mc08]. shifting [CPFL02, HRG07]. shifts [CPDZH08, FVY08, FFH+01, FO04, HWFN01, HLL06, Kae03, KKS04, LFS+07, LKA01, VBS09, WFH01, WHP02, WZXY07]. SHOP [YXC+07]. SHOP-type [YXC+07]. Short [TY05, GP05, HGMB04, IKYM09]. Short-range [GP05, HGMB04]. Short-time [TY05]. shorter [MST+08]. Si [BSB05, TK08, WZZ+09, YHD+06, CJ03, SURG06, WL09b]. sialic [UNHYT06]. SIBFA [PW08+03, PW08+04, ROG00]. SIBFA-LF [PW08+03, PW08+04]. side [DLH06, ENM+04, GT03, HFL06, JPF+00, KG02, LL01, MT03, MML05, PFC03, SMG09, VM02, XL07, Z06]. side-chain [ENM+04, GT03, JPF+00, KG02, MT03, PFC03]. sieve [PHH+08]. sieves [LMV07]. Sif [LAT05]. sigma [JFG04, KMM07]. sigmatropic [LL06, LFS+07]. SiH [ZZL+09]. silastannation [WCHW09]. SiLi [XFF06, HXD08]. silica [SDCG02]. siliceous [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, ZZT09, dGWH01]. similarity-based [RSS09]. similarity/dissimilarity [hyDN+08]. Simple [MO01, Ste04, ACLD03, Bac04, BLMS08, GRO+03, GD03, Gon07, ILB03, IT03, KS02a, LLW09, MCF05, SF05, BG00]. simplex [DV02, MCF05]. simplex-annealing [MCF05]. simplified [OH05, WC0+03]. simulate [LAEL01]. simulated [ADM+06, AB08, CCP04, HPP00, RLP08, WM06, WG02]. Simulating [Fie02]. Simulation [FBGD06, WWL+09, BBHD04, BVW04, BG07, BBM+09, CDD+05, CV09, CBH+05, Dra00, EA06, EMP07, FHR07, FEV+09, FPB+05, GS02, GJK00, HN02, HL09, IT05, IM06, IKYM09, IO02, JG05, KS+00, KB09, KEM08, KPR04, Kri09b, LM09, LEV+09, MLG04, MMMY07, MLV+05, MLCD01, MST+08, ON07, OT09, Pin01, PHH+08, SO07, SL06, SD07, TY05, VHRR07b, WEE01, XKG+05, YAC+02, YTH+07, ZALMG03, ZWTP+08, ZL09b, ZSK07, OBB05]. Simulations [FCP+05, MZL08, ATMK03, Ano06c, BWE05, BRDC02, Bie04b, BSJ01, CLO09, CIWL09, CJC09, CCS00, CF06, CPC+00, CEP07, CMD+04, CBH+03, DFF+05, DL09, DFB09, Der00, DSS03, DWC+03, ESM06, FGR07, FG02, FCP+04a, FAB+00, FC06, FKZ09, GL04a, GLP08, GW08,
GHH07, GS03, Gon07, Haf08, HB09, HGMB04, HHHS01, HH04, HM02, HPL03, Hin00, HFS03, HTKG08, HTSR04, HTN03, HMD06, IC08, JNV08, JCL05, JZD+09, KMH02, KFZ03, KM00, KKC05, KAK+09, KvGH01, KH06, Kri08, Kr03, KBN02, LML+00, LS004, LGB+09, LM03, LPB03, MB00, MFB04, MN02, MABM09, MBC08, MO09, MG00, NK01, NL07, Ni09, NO06, OR05, PRKP05, PHJ+08, PB04, PMB04, PK04, PB02, PNG08, RPMP03, RSER09, RMHK03, SK09, SDL+09, Sch04, SBG+09a, SWR06, SR09, SDM02, VCM01. simulations [VHRR07a, VP09, WL09a, WCF04, WZW+06, XLZ08, YNZ+08, YGLvG06, ZCS04, ZSC05, ZGFL01, ZWS+09, ZWZ09, ZSK07]. simulator [JGVF05, KIM+09, MS04, SO07]. simultaneous [DDVD09]. Singh [JVVK09]. Single [OV03, BG07, CV09, HSF08, IT03, IKYM09, LFZS04, WTKM06, XLZ+09, ZvRSC09, Mak08]. single-family [WTKM06]. Single-nucleotide [Mak08]. single-sphere [LFZS04]. Single-step [OV03]. single-walled [XWL+09, ZvRSC08]. singles [IN08, WKYU01, dSVA+09]. singlet [BLO+02, CZ05, CG08, FG03, LS08a, OSA06]. singlet-dioxygen [BLO+02]. singly [HHWG08]. Singular [FPG+06, TBSM09]. Sir [Ano04a]. Site [CJW+09, LLL07, AG00, CFR06, CFS+09, CF04, CFC+08, FPN+05, GJK00, GS04, HFS+07, HYR06, KSK00, KEB04, KZRO03, MDA08, NL07, NLL+09, PMM06, SS05, SRT+03, SFR07, TDH06, XLZ08]. sites [APG05, BSDM04, CLXC02, CLS+09, FPN+05, FSS00, GDV03, HM02, HLT+05, MJHS06, PXP01, SEKS09, SLC+09, Tie09, Wou00]. six [GJK00, NL07]. six-site [GJK00, NL07]. sixth [CGB+09]. sizable [CAG07]. size [BSOB05, EL09, HLLT09, KS02a, KH06, NK06, OBB05, OV03, YAC+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, KvGH01, Leh06, LZA02, Oos09, PO03, PBZ00, PBS01, RR09, RZWS07, SH07, TYO+02, Van02a, WS02b, ZP03, ZOJ+06, ZX09]. small- [SHH07]. smallest [SRS07]. SMART [TTBM09]. SMART-based [TTBM09]. smooth [GPN01, KSY+00, PZS04]. smooth-particle [KSY+00]. smooth-permittivity [PZS04]. smoothed [LV08]. smoothing [HPP00, ILB03, WS02a]. snapshot [YNZ+08]. SnCl [RD00]. sodium [FL07, MHS05, YS09]. SODOCK [CLH+07]. Soft [yChMnY08, ASDP+06, TLK00, TJE03, TGGP+00]. soft-core [TLK00, TJE03]. Software [Ano04b, BACJCT01, DvL01, Gly06, JVV09, CHB+05, GBP05, KBA+04, MMP+07, NSU+02, BLM08]. solar [KS05]. solid [CFS+08, CCC09, CMA+08, EGSS00, Ish02, KCK+08, SK05]. solid-state [CMA+08]. Solids [vDSSvA04, JB04]. solubilities [SHH07]. solubility [BBG+04, EDA04, KEH+02, LLW+09]. solute [BRLS08, BRLS12, FCP+05, LFZS04, MR04, YL09, ZS07]. solutes [BL+06, HMS06]. solution [ABWT09, BH00, BP07, BISB02, BH03, CP00, CCK01, CRSB03, DA01, EK06, ELK+09, FHRR07, FG02, GMA04, HH03, HMWC03, HSWN01,
solution-phase [TDH06]. solutions [Blo04, CPJ01, Loe03, PK04, VP09, XZ04, XZ05, ZWP08, LR03b]. solvated [HTSR04, HRR05, KHY00, QSS01, RSP03, BSC⁺01]. Solvation [COL01, HHP04, WB04a, WB04b, WB05, WD04, BCIB05, CRSB03, CCT⁺03, COL⁺06, DVO2, DHW⁺00, FOL⁺04, FBL08, FZL⁺06, GS02, GS03, GPN01, GWS⁺02, HC08, HLMR06, IV04, IvSV06, KIM⁺09, LF04, LFZS04, LS08b, MGL03, OVMV04, PZS04, PPYS08, RSE07, Sch00, SDL07, VM02, VP09, XL02, ZFL⁺05, ZFL⁺05]. solvation-effect [SDL07]. solvatochromatic [XZ04]. solve [KvGH01, XOW⁺00, Zho06]. Solvent [BA03, BA04b, SMA0V00, ZP03, ZGFL01, AG03, BHW00, BBHD04, BMLV04, BRLS08, BRLS12, ENM⁺04, FEVM01, FC06, GZL02, GL04a, GP06, GB04, HHS⁺05, HN02, JS07a, JZD⁺09, KIFK07, Kr003, KKS04, Lab08, LRI⁺02, LFBSK07, LS04, LL01, LFR⁺04, MBC08, MM07, MCM04, MS01, PMB04, RRZA08, RP07d, SBLK01, STSF02, SHSF05, SL06, TJE03, TSMNG01, Tot04, VBGL⁺00, WB04a, WB04b, WB05, WWL⁺09, YTY07, YXZ⁺04, YL09, ZCL09, BA04a, FZL⁺06]. solvent-accessible [BHW00, BMLV04, HHS⁺05, TSMNG01]. Solving [FS00b, Hof05, BF04, CCL06, CF04, LMJ02, SATO04]. Some [VE09, FMP08, JARM02, KCL06, McD08, Rao00a, Sch03, WL04, YLL⁺09, CMA⁺08]. sometimes [BE06]. Song [JW12]. Sons [Bic09, Lip00]. source [CSV⁺07, GCB03]. soybean [TGLL07]. sp [NYK⁺09]. space [Bie04a, BMTS01, CS01, CcG08, Ckt⁺08, CA03, GT03, HXL09, JO02, KF08, LcKL05, LJKL08, Nak02, NA06, OFK09, PRR⁺05, PB07, PB09, PRSMM02, QNF09, Sch04, THHN01, Van02a, YL06]. spaces [JHPRSM⁺05, PRSMM02, PRT⁺07, PRT⁺08, RSS09]. spacing [ZvRSC08]. spanning [SN00]. Sparkle [FRS05]. Sparkle/AM1 [FRS05]. Sparse [SSB⁺03, AGSFAL05, LEK07, RS05, RRS07]. sparsity [JS07]. spatial [Bie04a, Bie04b, RP07b]. special [KAK⁺09]. specialized [H05]. species [CFC⁺08, DR09, GHLK⁺02, HBM06, KZY09, WG02, YIN03, LMGR05]. Specific [FAR02, LR03a, BS08, HLT⁺05, Pin01, PR02, SFRS01, TGLL07, TST⁺08, UHN09, WCF04]. specificities [PB06]. specificity [CJW⁺09, DLRZ09, LLL07]. specified [Fau01]. spectra [Bac09, BACJC01, CNN07, CG08, Gor01, HKHN08, JARM02, KŠ09, KFD06, LDL⁺09, MLC00, NRHK02, OBB05, OKE⁺02, SBL05, SN06, TDH06, WM01, YXX⁺04, ZGXX06, ZWTP⁺08, dGW01]. Spectral [II02, CVR08, Gds τM⁺07, LFZS04, NINAT⁺07, NAT07, SMK00, WG02, ZSK07]. spectrometric [KZW⁺05]. spectroscopic [An006a, FCW06, KCL00, ST06]. spectroscopy [ACM⁺06, RDM⁺08, VDM06, WMRW⁺01, ZPL07]. spectrum [EL09, LMCD09, MWL⁺08, MGLD00, PRSMM03]. Speeding [KVF⁺07]. speedup [BYQ03]. sphere [HdMdS05, Hsd06, 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 [PSDM00]. splittings [HLLN06, SFRS01]. 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 [PSDM00]. splittings [HLLN06, SFRS01]. Spontaneous [Sza08]. square [CSB08, LLZL09, Nil09]. square-planar [CSB08]. squares [CSD05, Gol09]. Sr [WD08, SCP08, XBO8]. Sr-doped [SCP08]. SrFeO [Hua09b]. SrZrO [SM06]. SSB [KVS+06]. st2nmr [PRJ02]. stabilities [ACM+06, CTFC08, GYCZ04, STC+08, WDXS06]. Stability [JD09, Owe05, PHFC04, WSC09, CJS+03, CF06, DB07, HXD08, JS07b, JBGK08, OCP02, PGC05, QBO5, XFF06, ZXYF09]. Stability [JD09, Owe05, PHFC04, WSC09, CJS+03, CF06, DB07, HXD08, JS07b, JBGK08, OCP02, PGC05, QBO5, XFF06, ZXYF09, ZOJ+06, ZM06].
Stabilization [EBDPM00, HYA02]. stabilized [HSF08]. stabilizing [GZ07]. Stable [HDO+02, GYR06, KRLD09, KRM+02, LB08]. stacked [RRCA08, SB08]. stacking [CM09, DDBP09, HWTL03, KKY01, WR+06]. standard [ASDP+06, CG06, FBDG06, KOFF09, LFSB03a, LFSB03b, SSS+09, SL04]. standing [KDG+09]. staphylococcal [JS07a]. Starting [VZVG06, BWI+02]. state [Ang09, BB1+09, CWY09, CFS+08, CHA+07, Chu07, CAG07, CMA+08, HM01, HNW07, HNW12, Hin08, HP05, IME02, JHZ09, KTO2, KRI09a, LMK01, LZ05a, LDL+09, NTH09, PO03, PSS+04, POJ01, Qua07, SPS08, Sen06, SRE08, TH02, TST+08, TY03, TKN+08, WCFH02, WHF08, ZHO8, ZOJ+06]. state-speciﬁc [TST+08]. states [Ang09, ABBC01b, BOF01, BON01, CWY09, CNN07, DHM+03, DF04, EL07, FCW06, FDSA00, HFS+07, HYR06, ZH09, IR03, KUB07, LS08a, LXW07, LB09, MW09, MLCD01, NBTN04a, NBTN04b, OSA06, PRSMV08, Qua01, SBI08, SMK00, VW00, WLL+07, XZ05, ZL05, ZL07, ZL09b, ZM03, dSVA+09, ABBC01a]. static [FR08, LGD02, MAR03, XWL+09]. stationary [SK09]. Statistical [HFS03, PYEA03, DW08, EC06, KOB03, ML00, RK05, SB08]. statistical-thermodynamic [RK05]. step [BYQS03, BCP03, DLDW06, KM00, KH06, MK02, Mck07b, OVO3, OOS09, ZWZ09]. step/particle [BYQS03]. stepwise [LLKC06, LFS+07, NSB08]. Stereodynamics [CML05]. Stereoelectronic [DD08, PBF09]. stereoisomers [PCMG09]. stereoselective [AGI+00, AGI+07]. Stereospecific [PF06]. Steric [PF09, BDW00, XYN+06]. steroids [AGMPRG+08]. sterols [CSU05]. STFs [DBS08]. stiff [ECA06]. stilbene [CJK+02]. STO [CGB03, RRLR01, RLER05]. Stochastic [ARG03, FAN01, KEM08, SBN04, AM09, CS01, DH+05, GDSaM+07, MKT04, ZZ08]. Stoner [SK08]. stool [FKS+09]. storage [FR06]. stored [AT02, MBWP03]. stored-integral
[MBWP03]. Strain [ST01]. strained [ST01]. strand [GAS04, JS07b].
strained [AZM03]. Strategies [DBS08, LJS05, YL09, EKB02a, KEB04, Vis02]. strategy [BME05, CZA03, LLL08b, MCF07, R08, SMGE08, Wan09, WS02a].
streamlining [VGB08]. strength [DMJ05, FO08, SEKS09]. strengths [RM07]. stretch [Kle03, SDCG02]. stretching [CPDZH08]. strictly [FMSA06, TT01, TT05]. Strike [Ano06c, WZW06].
string [Qua04, Qua07]. strong [LC07, PGG06]. strongest [VHRR07b]. strongly [ONHN00].
strontium [RD06]. Structural [CZFH07, EM03a, CKA09, LWLS07, LFR07, MS03, BCP03, CKR08, CLF09, ECM+03, GZ07, HYA02, HHP04, KZY09, Kar06, KPK06, LL07, LJS05, NAT07, OFIK09, PK04, QLHL09, SL07, SVV+08, SRB06, XSHC06, XLC08, ZLS03, ZWP08, CA07b]. structurally [AGMPRG08]. Structure [BMTSC01, CDL06, HHGW08, HRR05, HS07b, ITS05, KCL06, KPR04, MN02, PGC05, PLC08, PHRR08, RG08, SG07a, AJ03, AGSFA05, BED02, BS01, BAH02, BA07, CLC03, CMB07, CDS09, CSD09, CMaGL04, CJS03, CN05, CLA00, CPUGD09, CSV07, DP03, DHH08, DHW09, Fau01, FL07, FL0D07, FCP04a, FL08, FLK07, GBL05, GT06, GGGL05, GdAcV07, HHJ03, HEP02, HN02, HP05, ILK09, JCA02, JLFH03, KP05, KFN08, KHY00, KOFF09, KKB01, KMB08, KIF07, KWK00, LD06, LEK07, LJ0L08, Loe09, LLL07, MOP07, MM00, MLL08a, MM02, NK01, NYH02, NCO05, OS08, PD02, PSCD09, PJB07, PM05, PJ02, PF06, QB05, RPN07, RI07, RS05, RRS07, SSB03, SJJ04, SB01, SCP08, TD08, TT01]. structure [TG05, Van02a, VHR07b, WZY04, WMRW01, WD08, WS07, XZ04, YXL09, ZZY07, ZZZ07, ZZ08, ZLD09, Z08, vDSSvA04, vEMK01, vE01, RRCA08]. Structure-based [BMTSC01, HS07b, KBK01].
Structure-breaking [HRR05, VHR07b]. structure-properties [CDGS09, CSD09]. structure-property [JLHF03, PSCD09]. structured [DC02].
Structures [AB00, CTFC08, HDX08, KS05a, PCMG09, RSSK03, Ama02a, BK08, BSP06a, BS05, BRV07, CUSS03, CS05, CRB03, D08, DF04, DSB02, DB02, DJB02, EBA07, FOL04, GYC04, JL07, GCC04, HM01, HK09, Hua09a, Hua09b, IG03, Kar01, KAS07, KKM04, LD05a, LW08, LLL05, LhWX07, LS05a, MKG06, Mas01, MHT01, PYCD03, PYS05, RO08, RSR09, RM00, RRS09, SO07, SHBD05, SW05, TZ01b, TZ01a, T08, TD06, VV02, WS05a, WB04a, WB04b, WB05, WDX06, WS02b, WS07, Wu06, WWS07, WM01, XFF06, XLZ08, YIN03, YW05, ZCL09, ZXY03, ZGX06, ACM06, FZ07, STC08, UM03, ZXL04, Z09]. studied [AGO02, CFC08, D03, HFS07, KMB08, LML00, RGP07, RJJ06, Sen06, SRE08]. Studies [JW12, ZWS02, AB00, AD06, An06a, BY06, BPC01, BI06, BS01, BMTFR08, CBM08, DBS07, EBA07, FK08, GYC04, GC04, JK00, Han01, HSWW00, mjZyL08, KCL06, KWK01, KKW02, Kle02, KZW05, LKT04, LWLS07, LDY08, LJ07, LF02,
LWY\textsuperscript{+}09, LSY02, MCR08, MK02, MOP\textsuperscript{+}07, MW00, RPNJ07, RZWS07, SGPS09, SS00, SWBM08, SJI\textsuperscript{+}04, SLL\textsuperscript{+}04a, SLHW09, SFR07, ST06, TJM\textsuperscript{-}03, TMBM02, TCSM03, VS02, VMA03, VL00, VS08, WLL01, WLS04, WLL\textsuperscript{+}07a, WyLG\textsuperscript{+}09, WLL\textsuperscript{+}03, WXX03, WCL05, WZXY07, WXK08, XL\textsuperscript{-}02, XKKL03, YIN03, YFR05, YLWL09, YLL\textsuperscript{+}09, YK09, ZDS\textsuperscript{+}05, ZWL\textsuperscript{+}05, ZZ\textsuperscript{+}06, ZAT07, ZXY03, ZL05]. \textit{studio} [Gan09]. \textit{Studt} [Ano06a]. \textbf{Study} [LSAS01, SBL05, YZ06, ZCS04, ABYM08, ASDP\textsuperscript{+}06, Ama02a, Ama02b, ATH\textsuperscript{+}03, AVB00, AZM03, BAL\textsuperscript{-}01, BTP09, BSB05, BISB02, BLO\textsuperscript{-}02, BRLS08, BRLS12, Bor03, BSS08, BGC\textsuperscript{+}09, BBI\textsuperscript{-}09, BZL05, CMLS05, CC07, CFS\textsuperscript{+}08, CUS00, CU01, CUSS03, CJS\textsuperscript{-}03, CFA07, CZFH07, CCCJ09, CJW\textsuperscript{+}09, Che01, CN05, CNO07, CSB08, CFD03, CFD04, CPUGD09, CJPZ08, CMD\textsuperscript{+}03, DGD\textsuperscript{05}, DLR\textsuperscript{+}08, DWS\textsuperscript{+}09, Der09, DMC05, EA08, EFA01a, FL07, FC06, FD03, FO08, FKU\textsuperscript{+}05, FKM\textsuperscript{06}, FKM\textsuperscript{+}07, FKS\textsuperscript{-}09, GXK09, GHLK\textsuperscript{-}02, GD09, Gog08, GM01, GLRL02, GGGL05, GD06, GKT04, GBBH09, HWFN01, HLLS05, HSF08, HELM09, HSMT04, HM08, HPLO3, HK07, HJCP01, HHP04, HLMR06, IB04, IV04, IvSV06, IJK09, mjIzsLyL07, JH09, JW00, JF0404, Kan04, KWHH07, KFD06, KSN01, KIFK07]. \textbf{study} [KS01b, KKMMS04, KS05c, LD05a, LMK01, LKJ\textsuperscript{-}04, LPK07, LWK08, LMC09, Lee09, LZA\textsuperscript{-}02, LL01, LJ03, LW04a, LX07, LXW07, LL\textsuperscript{+}08, LS02, LL03, LMMW04, LS08b, LLK06, LLW02, LKT04, LT\textsuperscript{-}02a, LT\textsuperscript{-}02b, LB08, LYZ\textsuperscript{-}08, LDL\textsuperscript{-}09, LMRV07, NTH00, NBTN04a, NBT05b, BPC01, HMMS09]. \textbf{substituent} [AGI\textsuperscript{+}00, AGI\textsuperscript{+}07, dVB01]. \textbf{styrene} [Ama02a, Ama02b, XPW09]. \textbf{subspace} [FS00b, Har04]. \textbf{substance} [CCP04]. \textbf{substances} [ATH\textsuperscript{+}03]. \textbf{substantially} [RK05]. \textbf{Substituent} [JWB05, Lee09, PWF01, BCP01, HMMS09]. \textbf{substituents} [PSF\textsuperscript{+}08]. \textbf{substituted}
Substitution [ZS+07, BS05, JT06, LFBSK07, SOOF05, SSB07, ZWS+02].
Substitutional [FSS00].
Substrate [BMTFR08, LCC09].
Subtype [FTLV01].
Subunit [OON01].
Subunits [MML+06, PHFC04].
Super [BA03, BA04a, vDSSvA04].
Superatom [LWW+06].
Superatom [FTLV01].
Superconducting [MDI04].
Superexchange [WL00].
Superimposition [ZA07].
Superlinear [FR06].
Supermolecule [BA03, BA04a, vDSSvA04].
Superposition [COS01, CSD05, GRC01, GCD04, IO08, Mas04, VKP+08, VZVG06].
Supershort [XWL+09].
Supramolecular [AM07, CMaGL+04, Won09].
Surface [ABBC01a, ABBC01b, BMLV04, BL05, Bof01, BHH+09, CF06, DLD+02, DR09, EBL+08, GZL02, GCD+08, GB04, HHS+05, HG08, JBGK08, KHK+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, TSMNG01, TRS02, VP02, YHD+06, YJF06, ZCS04, ZSC05, ZCL09, ZGFL01, ZBS03, ZXYF09, ZGXX06, EKB02b].
Surface-doping [JBGK08].
Surface-generalized [YJF06].
Surfaces [ATH+03, BHW00, BWZ08, DLD+02, EKB02a, EKB02b, ENM+04, FKJ+01, GS09, HSF08, HHP04, IC08, IDMC09, JB04, KEB04, MCF05, MS09, PB06, RAK+09, SPD01, Sch03, Shao2, SBG09b, ST04, YJF06, ZBS03].
Surrogate [McK07a].
Surrounding [KGL07, Yos02].
Survey [HS07a].
SuSi [CA04].
SV [COS05, WG02].
SVM [YMT04].
Switch [SF07].
Symmetric [AT02].
Symmetry [PDC+08, PCA+08, BB08, CAGR08, FCP+04b, LWX07, SZW+05, WLPF05, Eil07, PV03, PTC01].
Symmetry-adapted [FCP+04b].
Symmetry-driven [PV03].
Symmetry-generation [Ell07].
Synergistic [GS08].
Syngas [YQH09].
synthesise [BBSS06].
synthesis [HLC09, PHR+05, WLL01].
synthetic [NH05, WG02].
system [BL00, HELM09, HRBKB03, IS03, KYL03, LHJ+06, LCGA03, LDT07, MM03, PGH+04, PRSM03, Rud05a, YOB+08, ZAT07].
Systematic
systems [AS00, BH00, BP01, BME05, BGJ01a, BWI02, CN03, CG06, CvG08, CCK01, CMGDAC+07, DXW08, DRMD03, Don08, DK01, EGSG00, Ell07, FZL07, Fan01, GLMV09, HT03, JCA+02, JTR05, JG03, KSS08, KKC05, KAK09, KBL08, Kle02, Kle03, Kri09a, LMJ02, LC09, LLL03, LDG02, MMLC05, MKGA06, MTB09, MM07, MS01, Oos09, RLDI09, RSN02, Rud05b, Rud05c, SRS07, SS00, SYY03, SWV05, ST01, TH02, TT08, WNL+09, WH03, YCXY03, YZ04, vdVGM00].

T [BBI+09, Lu09, PFJ+03, ZKZ+07, DLD+02, Ike04, KVS+06]. T-cell [KVS+06].

table [Kau07, Nil09, SRB06].

Tables [ARL01].

Tabu [MGJAARC00, SE07, SE08].

Tailoring [BG03, KKG09].

Taking [SN06].

TaN [ZHMW09].

Tandem [UNHYT+06].

Tantalum [Tie09].

target [FM00].

tautonomic [LS08b].

Tautomerism [YX+04].

Tautomers [HHWG08, PG04].

TcNE [GYMN07, TD08].

tCONCOORD [SD09].

tCONCOORD-GUI [SD09].

TD [CHA+07, SB10].

TD-DFT [CHA+07, SB10].

TDDFT [SL04].

TDHF [QCK01, QCK02].

Te [HKHN08, WWS07, HWFN01].

Technique [COS01, GKH05, KLM+09, SATO04, TS05].

Techniques [Woo01, You11, AM06, BC02, FSM09, KH05, PAT+09, PDS01, VE09, WSM+09, vGGB00].

Teller [Kri08, VDM06].

Temperature [FG07, JS07a, KT02, KGD06, MN02, TD08, XK08].

Temperatures [KK01b, TK08, WHH+06].

Tempered [BBP09, CVVB04].

Tempempering [SPT+07].

Templated [ST04].

Tensor [BZP09, BAA07, RI07].

Tensors [CDL06, KRM+02, ZLD09].

Term [JCHS07, SP05].

Terminal [KK01a].

Terms [Duk01, BMLV04, HP01, LAR+03, RP07a, YZ06].

Ternary [Don08, MM07].

Territory [Sha07].

Tert [Bac09].

Tertiary [CMLS05, PRJ02, PF06, SO07].

tessellation [LJ04, PTC01].

Tessellationless [Pom04].

Test [BCF+09, BUMCMRL00, BLN01, BE06, CF04, FMPS08, KTM02, SB08, SM03].

Testing [CMàGL+04, BG03, PZS04, WWC+04, WWC+05].

Tests [KSB+02, NGTB03].

Tetraammonium [CW02].

Tetraazanaphthalenes [CdML06].

Tetrachloride [DMN05].

Tetracoordinate [MMRH07, SRS07, Wan09].

Tetracyanoethylene [LH02].

Tetracyanoethylene-contained [LH02].

Tetracyclene [AS06, AS09].

Tetrads [MHS05].

Tetrahedral [LSY02, OBT09].

Tetrahydroimidazo [SPS08].

Tetrahydroimidazo- [SPS08].

Tetrahydrooxouranylate [ivSV06].

Tetramer [RCA08].

Tetraoxide [JW12, SLHW09].

Tetrapeptide [DSR+07].

Tetrapeptides [GKTS04].

Tetrazine [JW12, SLHW09, XZ04].

Tetrazine [JW12, SLHW09].

Tetrazino-Tetrazine-Tetraoxide [JW12, SLHW09].

Tetrazole [dSVA+09].

TGSA [GRCD01, GCD04].

TGSA-Flex [GCD04].

Th [NSO+07].

Their [Bac04, Bac05, Bac07, BWZ08, BHH+09, DVR+03, FL08, GCD+08,
thioamide-containing [LKJ+04]. thioether [SFR07]. thiolate [DMN05, SGD06]. thiomandela [APG05]. thiopeptides [TTB01a, TTB01b]. 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, Bie04a, Bie08, BGC+09, CV09, DHW+08, FII+07, FLOD07, GDV03, HK08c, KBLP09, Lai07, MP03a, MVLG06, SHBD05, Wan09]. three-body [FII+07]. three-bond [KBLP09]. three-center [Lai07]. three-coordinate [BGC+09]. three-dimensional [BP01, MP03a, MVLG06, SHBD05, 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]. tilit [LIH09]. TIM [AGK03, LD05a]. Time [Bac09, CP08, Gog08, Kol04, LLDF09, Whe08, ZH08, BYQS03, CJKF08, CPC+00, DF06, FCW06, HNWF07, HNWF12, HS01, IO07, KMM02, KM01, KH06, MW09, NTH09, PK05, PSF+08, TYN05, TST+08, TKN+08, YH07, ZWZ09, ZM03, vGGB00]. Time-averaged [CP08]. Time-dependent [Bac09, Gog08, LDL+09, Whe08, ZH08, CJKF08, FCW06, HNWF07, HNWF12, HS01, IO07, MW09, NTH09, PSF+08, TST+08, TKN+08, YH07, ZWZ09, ZM03, vGGB00]. time-frequency [DF06]. Time-reversible [Ko04]. time-step [KM00]. times [DDVD09]. timescale [MST+08]. TiN [JD09]. TINKER [Sto05]. TiO [FHRR07]. TIP4P [HPL03, THH01]. TIREs [LMGR06]. titanium [UNM+01]. Ti [VHRR07b, VHR007a]. TIX [ZL09b]. tm [BM00, GM01]. TMPyP [AZM03]. toluene [GCCV00]. tomography [RGGO8]. tool [ALB09, ACID+03, CCL06, CA07b, Gra07, HCHG+09, LAEL01, LOL+08, NSU+02, OLML+00, Pre01]. toolkit [Hna00]. tools [MRS09, Ney07]. topo [GRCD01, GCD04]. topo-geometrical [GRCD01, GCD04]. topological [CGR08, DRS04, DRS05, FSS00, GDPCPU07, HM08, JLFM03, MP03a, RP07c, RP07b, SFC04, YWHL03, ZE08, ZNLL07]. Topology [RSE09, FCP+05, GDACV+07, KLE03, KF03, KBL08]. Topology-based [RSE09]. Tork [CG03]. torsion [Ane06c, CIB05, FWH+07, FKZ09, MGLDS00, OMMH08, PRH+05, TNS00, WZW+06]. Torsional [PSF+08, DHI+05, FPG+06]. torsions [SP05]. total [RP07a]. toxicity [CMC05]. Tp [HT05]. TpMXO [HT05]. trace [KLS02]. tracing [KL01]. tracking [HNR08]. training [AG03, LJZ+07, LSY02, SJJ+04]. trajectories [Ham07, MST+08]. trajectory [Qua07]. trans [BZL05, CSB08, HKH08, KMM07]. trans- [BZL05]. transamination [LDY+08]. transcriptase [AJNG01]. transfer
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types [BY06, GGP09, KS05b, MLL08b]. Typical [SMV09, MLL08b]. tyrosine [AG00, CLS09, LRI02, Li01, LL01, OO08].

Typical [SMV09, MLL08b]. tyrosine [AG00, CLS09, LRI02, Li01, LL01, OO08].

U [Han01, CCCJ09, GHLK02, RLDI09]. ubiquinone [IN01]. ubiquitin [KIFK07]. UCSF [PGH04]. ultra [DHW00, HdMdS05]. ultra-incompressible [ZHMW09]. Ultrafast [BR07]. ultrasonic [PSS04, PSMB05]. umbrella [RNG03]. unbiased [SY09]. unconstrained [DMN03]. uncorrected [PSC01]. understand [DSB02]. Understanding [CAGR08, CDPL09, BRS07, ZZW09, CFER04, HP04]. Unicorns [FK07b].

Unicorns [FK07b]. unphysical [OV03]. UNRES [HXLS09, NCO05]. unrestricted [YH07]. unsaturated [BS03, KFD06, MTB09, Wan09, ZKZ07]. Unusual [XK08]. UO [IV04, IvSV06, RDM08]. Update [BKS02]. updated [Chn07]. Updates [Ano04b, BACJCT01, DvL01, Gly06, JVVK09]. upon [OFIK09]. uracil [LMGO09, MSBS01, MHS05]. uracil-base [MHS05]. uranyl [IV04]. Urea [SK05, AS00, VVS07]. ureases [ESM06]. Use [BWI02, DW08, Wou00, ALB09, FC06, JNV08, Kl01, MRC03, OPC02, PRK05, PRS04, RCJ02a, RSN02, Ruv07, SH07, SVT09, VGMM05, YTH01, YZ04]. used [DvG00, ESP04, HdmS05, HdS06, HD06]. user [DPDG05, JKI08]. uses [KBB09]. Using [CSD04, FSM09, HL08, Kac05, LL07, MO01, OSH03, QLH09, SWR06, XSHC06, XL08, XOW00, Ade04, AJ03, ABWT09, AM06b, AS00, BW07, BMLV04, BVW04, BME05, BGC09, Bud07, CLW09, CN03, CSJ01, CLC09, Ckr08, CLA0, Chn07, CP08, CPO09, CCP04, CPML08a, CGSD06, DLD02, DWB01, DRO9, DVP02, DB06, DB02, DMJ05, EKO01, EKB02a, EM03b, FCW06, FMPS08, FBG06, FAB00, FEV01, FR06, FSF05, GMA04, GL04b, GdSM07, GPSP06, GGLR00, Ha08, HWD03, Han01, HSM04, HMM06, HMM09, HG08, HHP04, II02, IS07, IS03, IT03, IK00, JBC08, JIK09, JVVK09, JTR05, JFG04, JSH07, KRM02, KKG09, KM00, KLM04, KK08c, KOFF09, Kle02, Kleeo3, KBT03, KKS04, Lab08, LCKL05, LCC09, LZO5a, LLL08, LZZC09, LS05a, LZ05b, LS02, LKW04, MWL08, MT03, MMLC05, MKT04]. using [MV06, MBP09, MOP07, MTE04, MRS09, MRS07, NCO05, NINAT07, OFB08, OKE02, PMB04, PS09a, PAT09, PP08b, PDS01, PZS04, PSS04, R107, RI08, RMP01, RG08, RON02, SDL09, SPGS08, SSB03, Sch00, SRC03, SBG09a, SY09, SPT07, SMV09, TP01a, Tie09, TCSM03.
v [Lip00, ZZW09, GBJ03, Kri09b, PFC03, TD08]. vacancy [ZMH+09].

vacuum [BISB02]. Valence [LW07, Sh08, Tru07, WM12, Bie09, BLT03, Cui08, EA08, HELM09, HS07a, May07, MG00, PRSMV08, SWZS04, SMZW05, SSMMW09, SSW+07, VBGL+00, WMRW+01, WJ00, dSVA+09, vLBBR12]. valent [AZM03, CN05, GSWL07]. validation [BAA07, VCM01, AGI+00, DGD+05, JJB02, JCL05, JVVK09, MSR04, SRB06, APG05, HZ06b, NGTB03]. valinamide [HCP01].

value [FPG+06, TBSM09]. values [OS06, PMPGP05]. vanadium [PV07, Tie09]. vapor [PHJ+08, UNM+01]. variable [CFS+09, GS08, WHRG08]. variables [SWR06]. variance [Blo04, LRWG03]. variate [LR06]. Variation [AAP00, NAT07, PGG06, Rao00a, Vya01]. Variational [MR02, AB09, Chu07, GY06, HDMdS05, HDS06, HD06, RS07a, RS07b]. Variations [TGGP+00]. variety [SBL05]. various [BP07, HMMSS09, IT03, Kr0603, KSS01b, MLL+08b, PP08a, PFJ+03, PML05, RR05, WHH+06, ZCL09]. varying [CC09]. VASP [Haf08]. VBSCF [vLBBR12]. VCH [Sta00]. VDD [GHB04, GHB04]. vector [CLXC02, CLS+09, HL08, LCC09, LJJ+07, QHL09, YMT04]. vectorizing [SO07]. vectors [BWI+02]. versatile [KF08, TdMSD+08]. version [HD04, LRWG03]. versions [Sto05]. versus [ABYM08, LAC08, BSG07, BB08, JS07b, JBGK08, LST08, LTV08, PSM05, Van02b]. Vertical [PRSM03, SA07, CG08, IWX07, LFEdL06, SLRC01, TKS+01]. VI [HP05]. via [BA03, BA04a, Bou01, BR500, BRS01, CZB07, CAG07, DFGB09, Hua09a, JP09, KSB+02, KRLD09, LMO09, SMM+08, SG01, ZPL07]. Viability [KK01b]. viable [LMGR05]. Vibalizer [Gra07]. vibrating [Yos02]. vibration [CCL06, LSY02, ZWP+04]. Vibrational [BP07, CLP+05, LC09, NR04, WB07, BRV+07, DB07, GBDP05, Gra07, Han01, HNR08, JARM02, LMB08, LN01, MR02, NRK02, NAT07, PZWG+04, Tor02, WM04, WM01]. vibrations [CPDZH08, DR09, KCL00, vE01]. vibronic [TP01b]. view [CSJD04, Jac09, JMD+02, MGCA07]. VIII [EBD+01]. vinyl [YYW07]. vinylphosphine [MGLS00]. viridis [IN01, OON01]. virtual [GS05, KSM05, LZ05b, PRDS08, YOB+08]. virus [AJNG01, DLRZ09, KCL06]. viscosity [ZP03]. Visualization [MMP+07, RP07b, ARL01, KYL03, PGH+04]. Visually [SD09]. VMD [Pra01]. VMFCl [CCL06]. VO [PV07]. voltammetry [KJP+07]. Volume [Sta00, BVW04, Lab08, LFS03a, LFS03b, Mue01, QNF09]. volume-preserving [QNF09]. volumes [BHH+09, Rao00b, SBLK01]. Voronoi [GHBB04, MVLG06, SBLK01]. VP1 [KCL06]. VPP700 [KSY+00]. Vpu [KF08]. vs [CXZ+09, LLK06, MA05, SCG04, Wib04].
W [UM03, WW05, MH09]. W2 [dOMSL01]. Waals [AD00, CPUGD9, GdSuM07, Gri04, KLB04, LS08c, VS02]. walk [CY09, CY13]. walking [BHG03]. wall [BG07]. walled [XWL09, ZZvRSC08]. Wang [Ano06c, GHH07, JW12]. warping [JO02]. Water [LMIF06, Mor02, NK01, BUMCMRL00, BRLS08, BRLS12, BSH07, CCK01, CSB03, DLR08, DSB02, ES00, FG03, FBGD06, FK80, GWM08, GDV03, G09, H02, HRKB03, HPL03, HFI06, HN02, HTN03, HLMR06, HT04, LS08c, VHRR07a, VHRR07b, YS09]. Water-addition [RR05]. Water-assisted [BA04b, WJX08]. water-phase [KFNH08]. WATGEN [BSH07]. Wave [GBJ03, Bac04, Bac07, Bou00, GFS05, MLL06, PFB05, PPYS08, RR05, SO07, SSM08, SJM09, T04, UM03, VHR07a, VHR07b, V00, W00, WD04, W07, XXK05, YS09, YS09, YGLvG06]. Warping [JO02]. Wavefunction [IS07]. wavefunctions [BWW08, KTM02, PJPjdPRMI07]. Wavelet [CF04, ON07, QLHL09]. waves [MBH07]. weak [QTdG08]. weakly [CPM08a, JRJ01]. web [KKG09, Gra07, JKI08]. Web-based [Gra07, JKI08]. web-interface [KKG09]. WebMTA [KKG09]. WebProp [GKRG08]. Wei [Ano06c]. weight [AG00]. weighted [FS00b, HWDB03]. weights [Bac04, Bac05, Bac07, Kar01]. Weinhold [GHBB04]. well [BBP09, WKC00]. well-tempered [BBP09]. where [HYA02]. which [SBH02]. Wiener [YWH04]. Wiley [Bie09, Lip00, Sta00]. Wiley-VCH [Sta00]. Will [LLW09]. Windock [HS07b]. Windows [HS07b]. Windows-based [HS07b]. wise [Nil09]. within [Der09, FDM00, GS09, KC01b, MY08b, NYTH09, NAT07, SBD05, SPT03]. without [AL01, HD06, HD06, HZ09, Nil09, PK05, Qua07, RKA09, TW03]. WNO [HT05]. worker [FCK08]. worker-based [FCK08]. Working [Nye07]. World [Woo01, You11, FKB07]. worlds [Sim07]. Wu [Ano06c].

X [BAL01, BPC01, CRC08, Dib05, HZ09, Hua09a, KBL08, LS08a, Mck07a, Mck07b, S08, RB01, STL08, WLLS04, WZZ09, WWS07, ZJM07, ZY01, ZLO9b, HYA02, HS01, TN02, LP00, Mar03, Sta00, WKU01]. X-ray [HSSW01, HN02, WKU01]. xanthate [CFD03]. XCu [KBL08]. xenobiotics [PCMG09]. xenon [HS06]. XES [EKO01]. Xiang [Ano06c]. Xinli [JW12]. XMVB [MZW05]. XPS [EKO01]. XX [CRC08]. XXIII [PFJ03]. XY [Z01]. xylose [GVATG03].

yield [CSD05]. YL [NYK09]. ylide [LS08b]. ylides [Mit01]. Ylidic [XDS06b]. yloxy [BE07]. Yong [Ano06c]. young [SN00, W00]. ytterbium [FRS05].
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Yuzlenko:2009:MMA


Yang:2006:GAP


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**Yu:2007:PRI**


**Ytreberg:2004:EUN**


**Yang:2006:SPC**


**Zhu:2007:SOS**


**Zanuy:2003:TIP**


**Zheng:2007:CSS**

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<td>[ZGXX06]</td>
<td>Zhu, Guo, Xue, and Xie</td>
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**Zhu:2007:CIS**


**Zhao:2008:TDD**


**Zou:2009:HPQ**


**Zhao:2009:FPI**


**Zhou:2006:RCP**

Zeng:2007:EAH


Zhao:2007:CDQ


Zou:2005:ETS


Zou:2007:TSL


Zhu:2009:NME


Zou:2009:CIC

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Zhu:2008:ISE


Zhu:2009:SPH


Zhao:2004:ACT


Zhu:2003:TSS


Zhang:2008:SIG

Zhang:2009:FPC


Zhang:2001:CRE


Zhang:2008:REE


Zhang:2004:DLI


Zhang:2008:TSO


Zhang:2009:TSR

REFERENCES


Zhang:2007:SEG


Zhou:2009:GSB


Zhou:2008:ICS


Zhang:2007:TSB


Zhang:2009:TUV


Zhang:2007:EPW

