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Title word cross-reference

(Φ, Ψ) [WD04]. (φ, ψ) [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]. $4d$ [ABYM08]. 5
[ZXL⁺04]. $5d$ [HZ09]. 6 [Han01, LLXS02]. 7 [LMO09]. 8 [KS05a]. 9 [UM03].
 $[n]$ [VKP⁺08]. $##$ [BRV⁺07]. $+$
[FKS⁺09, GLRL02, GPSP06, GWL07, HDO⁺02, ITS06, KT08, LMO09,
Mck07b, PV07, Sha02, WWT08, ZWY⁺09, ZL05, dRLMS00]. $+2$ [PNG08]. $-$
[Bac09, Dib05, HTN03, LYZ⁺08, Mas01a]. 1

[AGI⁺07, IS03, LDT⁺02a, XZ04, ZX04, ZLLS04b]. ¹²⁵ [HWFN01]. ¹³
 [FHF⁺01, VBS09, ZLD09]. ¹⁵ [LKA01]. ¹⁹ [FO04]. ¹ Σ [BAL⁺01]. ¹ Σ_g^+
 [BAL⁺01]. ² [BAL⁺01, Gog08, PRSMM03, ZWS⁺02]. ²⁺ [AS06, BTP09,
 BL00, FHRR07, GPSP06, HLB09, KRLD09, Kri08, ROG00, TFZRG01]. ²⁻
 [IvSV06, JD09]. ² Π [Gog08]. ³ [BPC01, LDT⁺02b]. ³⁺
 [BTP09, BL00, Kri09b]. ⁵ [WC08]. ⁵⁷ [HLLN06]. ^{α} [VBS09, CJW⁺09]. ^{\bullet}
 [Mui05]. ^{*ISQ*} [Bac09]. ^{*MTCP*}1 [BRDC02]. ^{*n*} [ZZZ⁺06]. ^{*p+*} [GPSP06]. ⁰
 [DLD⁺02]. ¹
 [BPC01, DLD⁺02, WLPF05, XWXC08, YKK09, ZZW09, XWXC08]. ¹⁰³
 [NSO⁺07]. ¹¹ [XB08]. ¹² [WZZ⁺09, XB08]. ¹⁴¹ [GYCZ04]. ¹⁸ [ZZZ⁺06]. ²
 [Bac09, BAL⁺01, BL00, BBI⁺09, CPJ00, CCCJ09, CTFC08, DLD⁺02,
 DRAS04, DRAS05, Dib05, DMN05, Don08, FJ08, GCCVB00, GBDP05,
 GPSP06, HYR06, HK07, Hua09b, IN08, IV04, IvSV06, IS03, JPF⁺00,
 mJlZsLyL07, KZY09, KS05a, KKJH08, KBL08, KS05c, LDMR01, LC07,
 LWK08, LLXS02, LW04a, LZCC09, LAT05, LF02, LDT⁺02b, LWY⁺09,
 LMO09, MR02, Mas01a, Mas01b, MGLL03, McD08, Mck07b, MY08a, NA06,
 NyHN06, NHN06, Owe05, PGNG03, PGRRNG03, PC00, PRSMM03, PLC08,
 RAGLL09a, RAGLL09b, RD00, RDM⁺08, SLL⁺04a, SLL⁺04b, SRE08,
 STC⁺08, TJM⁺03, TD08, UCT⁺03, UTT⁺04, VS02, WLLS05, WDWS06,
 WDS06, WLL07a, WDZS07, WLL⁺07b, WD08, XFF06, YTY07, YLW⁺08,
 YLWL09, ZY01, ZZL04, ZLLS04b, ZWL⁺05, ZLLS06a, ZLLS06b, ZKZ⁺07,
 ZXY03, ZX09, dOMSL01, dRLMS00]. ²⁰
 [Ber03, CCB04, Eli07, GB02, Var09, WLPF05, WL09b, ZZZ⁺06]. ^{\dagger}
 [dOMSL01]. ^{$\bar{2}$} [LMCD09]. ^{2^+} [GHLK⁺02]. ^{2^-} [GYMN07]. ^{$2A$} [YKK09]. ³
 [BPC01, CPJ00, DRAS04, DMN05, FJ08, GBDP05, GD06, HLLS05, HYA02,
 HDO⁺02, HTN03, ITS06, mJlZsLyL07, mJlZyL⁺08, KZY09, KT08, KKJH08,
 KSTC01, LDMR01, LD05a, LMK01, LDC⁺07, LW04a, LWW⁺06, LF02,
 LWY⁺09, MR02, Mas01b, MGLL03, Mck07b, Mui05, NA06, ON07, PGNG03,
 PGRRNG03, RD00, SAS05, SLL⁺04a, SM06, SCP08, TJM⁺03, TK08,
 TDK07, UTM⁺02, UTT⁺04, VDM06, WDS06, WLL⁺07b, WDX⁺02,
 XDS06a, XFF06, YLW⁺08, YLWL09, ZJM⁺07, ZZL04, ZLLS06a, ZZW⁺07,
 ZZL⁺08, ZXYF09, ZZL⁺09, ZKZ⁺07, ZWS⁺02, ZX08]. ^{$3-n$}
 [mJlZyL⁺08, KSN01, WLL07a, WDZS07]. ³⁶ [CS01]. ⁴
 [DRAS04, DMN05, IN08, IvSV06, JD09, LDMR01, LMK01, Mck07a,
 PHH⁺08, TYN05, TK08, UNM⁺01, UTM⁺02]. ^{$4-n$}
 [FHF⁺01, WDX⁺02, XLL⁺02]. ⁵
 [GD06, LYZ⁺08, SLL⁺04b, ZZL04, XWXC08]. ⁵⁰ [ZZvRSC08]. ⁵⁴ [GZ07]. ⁶
 [BSJ01, GHLK⁺02, Han01, KRLD09, LDMR01, LZCC09, LAT05, LYZ⁺08,
 RPNJ07, SLL⁺04b, TYN05, XB08]. ^{$6-n$} [Han01]. ⁶⁰
 [CJS⁺03, Eli07, KJP⁺07, Owe05]. ⁶² [HK07, STC⁺08]. ⁶⁴ [CTFC08]. ^{4^-}
 [CTFC08]. ⁷ [HYA02, LZCC09]. ⁸ [GZ07, Mck07a, Mck07b, PLC08, WLL01].
⁸⁰ [KSN01]. ⁹ [Mck07a, Mck07b, PLC08]. ⁹⁰ [NSO⁺07]. ^{*A*}
 [Sha02, KKS04, MK02, ZPL07]. ^{*cam*} [ZAT07]. ^{*carbene*} [HA04]. ^{*h*} [WLPF05]. ^{*i*}
 [OS08]. ^{*m*} [LYZ⁺08]. ^{*N*} [BP01, BSB05, HTN03, MG00, Owe05, RC04, YT04,

DRAS05, FHF⁺01, Han01, HXD08, mJlZyL⁺08, KS05a, KSN01, LLXS02, LMGR06, LMO09, Mas01a, Mas01b, QB05, TJM⁺03, UM03, WLL07a, WDZS07, WDX⁺02, XLL⁺02, ZY01, ZXL⁺04, ZXY03, ZGXX06]. *s* [WLL01]. *x* [KGL07, RAGLL09a]. *A* [Dib05]. *α* [CMD⁺04, CPML08b, FKU⁺05, IGNH03, KLS02, LZZC09, LDY⁺08, LLL07, MCF07, MML⁺06, PCO⁺07b, PCO⁺07a, RY09, SWBM08, SBG⁺09a, TFZRG01, Van08, WCF04, ZWPR⁺04]. *α*₃ [MH09]. *β* [AGO⁺02, APG05, BTP09, BCP04, BSP06a, CSJ01, CJW⁺09, CLA⁺00, ESM06, GTC06, GAS04, HL08, IGNH03, KF03, LLW02, MCF07, MML⁺06, MS03, MK02, PP08a, PGC05, PSF⁺08, PMM05, RMP01, SBG⁺09a, SDM02, TFZRG01, TK08, ZALMG03, ZHH09]. *β*₂ [YKK09]. *β*_{2m} [WCF04]. *c* [BS06, JKL08, KK01a, OON01]. *·* [VS02, ZY01]. *χ* [OMNH08]. *d* [ASS⁺02]. *Δ* [CFR06]. *ΔΔ* [AGI⁺07]. *η*² [KJP⁺07]. *η*⁶ [FKŠ⁺09, GM01]. *f* [ASS⁺02]. *g* [KRM⁺02]. *γ* [HL08, Ike04, TK08]. *k* [DLW06]. *λ* [CN03, KB09]. *↔* [UCT⁺03]. *m* = 1 [LYZ⁺08]. *μ*₃ [KJP⁺07]. *N* [BY06, CCK01, GSB09, HT05, HRBKB03, HJCP01, JD09, KK09, KKH⁺07, KK01a, MMPK01, ZPL07, MGMM07a, MGMM07b, VVBV02]. *n* = 0 [FHF⁺01, mJlZyL⁺08, KSN01, LLXS02, TJM⁺03, ZZZ⁺06]. *n* = 1 [Han01, KS05a, 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 [LMO09]. *n* = 8 [LMGR06]. *nd*¹⁰(*n* + 1)*s*⁰ [GPSP06]. *o* [OSA06]. *Φ* [SO09]. *π* [Ang09, BY06, CXZ⁺09, DMZT08, EFQD09, GYMN07, HIM07, IINK09, LC09, LFR07, MM05, OO08, RRCA08, SSS⁺09, ST01, WRP⁺06, Wou00, WJ00, YTH⁺07, ZGZX07]. *π*^{*} [Ang09, XZ04, ZX04]. *pK_a* [KK08b, SMG09]. *Ψ* [SO09]. *→* [Ang09, CMD⁺04, Gog08, HTN03, LW04a, MGLL03, PGNG03, SOOF05, SLL⁺04b, ZZL04]. *s* [ATM⁺07, GRO⁺03]. *s/d* [Hol05, SZT08]. *σ* [CXZ⁺09, HIM07]. *sp*² [TTB01a]. *V* [Ang09]. *x* = 4 [KGL07].

-1 [PWFS01, ZPL07]. **-2-chalcogena-trans-hydrindans** [HKHN08]. **-2-methyloxirane** [ZPL07]. **-34** [PHH⁺08]. **-acetaldehyde** [Lu09, Lu09]. **-adrenergic-based** [YKK09]. **-alkanes** [VVBV02]. **-amino** [CLA⁺00, LDY⁺08]. **-amyloid** [MS03]. **-arene** [FKŠ⁺09]. **-assisted** [KT08]. **-ATPase** [HLB09]. **-based** [JD09]. **-benzodiazepinone** [SPGS08]. **-benzylideneaniline** [BY06]. **-block** [ATM⁺07, ASS⁺02]. **-C** [KJP⁺07]. **-carbon** [KLS02]. **-carboranes** [OSA06]. **-center** [MGMM07a, MGMM07b]. **-channel** [CXZ⁺09]. **-cis** [GRO⁺03]. **-conjugated** [LC09, LFR07]. **-D** [BAH⁺02]. **-dependent** [PMM05]. **-di-substitution** [ZWS⁺02]. **-diketiminat**e [GTC06]. **-diketonate** [RMP01]. **-dimethylcarbamate** [KKH⁺07]. **-Dynamics** [KB09]. **-effect** [RY09]. **-electrocyclization** [ZGZX07]. **-electron** [BY06]. **-electrons** [WJ00]. **-formyl-** [HJCP01]. **-formyl-alanine** [GSB09]. **-formyl-glycine** [GSB09]. **-formylglycinamide-water** [HRBKB03]. **-glucans** [CMD⁺04]. **-glutamine** [WC08]. **-H** [LLL07]. **-Hairpin** [ZHH09, CJW⁺09, IGNH03]. **-Hairpins**

[IGNH03]. **-Helical** [CPML08b, Van08, PCO⁺07b, PCO⁺07a]. **-helices** [IGNH03]. **-helix** [JS07b]. **-hydrogen** [ZGZX07]. **-jun** [KK01a]. **-lactamase** [AGO⁺02, APG05, SDM02]. **-lactamases** [ESM06, MK02]. **-lyase** [PMM05]. **-maltotriose** [SWBM08]. **-mercaptocarboxamides** [TFZRG01]. **-metal** [Wu06]. **-methoxycarbonyl** [KK09]. **-methyl** [CCK01]. **-methylacetamide** [MMPK01]. **-methylimidazole** [HT05]. **-methyloxaziridine** [ZPL07]. **-Mn** [AZM03]. **-peptide** [BSP06a, CSJ01, CLA⁺00, ZALMG03]. **-peptides** [BCP04, LLW02]. **-phthalocyanines** [LS02]. **-pleated** [PGC05]. **-porphyrazines** [LS02]. **-quartz** [ZWPR⁺04]. **-R** [LZZC09]. **-radical** [CXZ⁺09, CXZ⁺09]. **-scaled** [CN03]. **-sheet** [KF03, PP08a]. **-Si** [TK08]. **-sigmatropic** [LLKC06]. **-SO** [ZZW09]. **-stacked** [RRCA08]. **-stacking** [WRP⁺06]. **-step** [DLW06]. **-strand** [GAS04]. **-substituents** [PSF⁺08]. **-TCNE** [GYMN07]. **-tensors** [KRM⁺02]. **-terminal** [KK01a]. **-the** [VHRR07b]. **-TMPyP** [AZM03]. **-turns** [HL08]. **-type** [OON01].

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

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

1 [AJNG01, AVS09, BPC01, BWE05, KF08, NLL⁺09, SPT⁺03, VVS07, WC09, WHF08, YT04]. **1-** [CUS00]. **1-amino-3-propenal** [FDSA00]. **1-jk** [SPGS08]. **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, PO03, RC04, WC09]. **2-allyl-2** [ZGZX07]. **2-amino-2-imidazoline** [XKG⁺05]. **2-amino-2-oxazoline** [XKG⁺05]. **2-amino-2-thiazoline** [XKG⁺05]. **2'-aminoarabinonucleosides** [BL08]. **2-Aminopurine** [SC01]. **2'-aminoribonucleosides** [BL08]. **2'-azido-2'-deoxyribonucleoside** [PFR04b]. **2-chloro-** [JKM08]. **2'-deoxyguanosine** [MM02]. **2'-deoxyribose** [LBG08]. **2-difluoroethane** [CUS00]. **2-dihaloethanes** [WFR08]. **2-dihydro-pyrimidinyl** [WJX⁺08]. **2-dimethoxyethane** [LCGA03]. **2-electron** [ABF⁺03]. **2-H** [LDC⁺07]. **2-oxazolidones** [OY01]. **2-oxo-1** [WJX⁺08]. **2-oxoimidazoles** [JKM08]. **2-phenoxy-carboxylic** [XKKL03]. **2-substituted** [OSA06, WW04]. **2-thiouracil** [LMGO⁺09]. **2.0** [GZM09]. **21C7** [GLRL02]. **21D8** [UTH⁺03]. **22** [Bof01, Qua01]. **24** [Ano06b]. **25** [Kne05, WB04a, WWC⁺05]. **26** [Ano05b]. **27** [Ano06a, Ano06c]. **28** [HNWF12, Van08]. **2B6** [LCC09]. **2B6-substrate**

[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]. **3D** [DHW⁺08, SGPS09, CGMPT⁺08, CPUGD09, MH08b, VB09]. **3D-chiral** [CGMPT⁺08]. **3D-RISM** [MH08b]. **3D-structure-function** [CPUGD09]. **3DEX** [SHBD05].

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

5 [LDY⁺08, PFR04b, PMM05, TAS07]. **5-di-tert-butyl-o-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** [MRS⁺07]. **67-residue** [MH09]. **6G** [VSW⁺03].

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

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

9-heterofluorenes [CZFH07].

= [Bac09, CPJ00, CRC⁺08, GHLK⁺02, GPSP06, Han01, HT05, HYA02, HKHN08, HZ09, Hua09a, JJK⁺00, KBL08, LS08a, LZZC09, LYZ⁺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, ZMZ09, BMRF01, DHF⁺05]. **absorption**
 [MWL⁺08, MSH⁺06a, YXZ⁺04]. **abstraction** [AST06, CUS00, CUSS03,
 GAIMVB01, mJlZsLyL07, LW04a, LLL07, TGLL07, WLLS04, XLL⁺02]. **Ac**
 [GHLK⁺02]. **accelerate** [Gon07]. **Accelerated**
 [LSG06, LDG02, FSM09, Har04]. **Accelerating** [FEV⁺09, LEV⁺09, SPF⁺07].
Acceleration [KG02]. **accelerator** [ATMK03]. **acceptance** [KBB09].
acceptor [BL06, RM07]. **accessibility** [AG03, ENM⁺04, GP06, Tot04].
accessible [BHW00, BMLV04, GB04, HHS⁺05, LFBSK07, RP07d,
 TSMNG01, TRS02, ZCL09]. **accessible-surface-area** [ZCL09].
Accompanying [Ish02]. **account** [May07, SN06, Vya01]. **Accuracy**
 [FII⁺07, GG09, PSMB05, SKK⁺07, UBDPJ04, Bie04b, FKFG08, JS07b,
 KC01b, MKGA06, MHW04, RK05, SM03, SW06]. **Accurate**
 [ABWT09, BdPRMAI00, EK06, GK09, Gri04, HdS06, HD06, HMSM06,
 Ish04, LLZL09, MSH⁺06a, Tot04, WFHP01, WHP02, WHF08, WX09,
 ALKH04, Bie04a, BLB09, CGBF05, CF06, GKK07, HdMdS05, JJK⁺00,
 Rud05a, Rud05b, Rud05c, Vas02, WCC08, ZFW08, vEMK01]. **accurately**
 [IGL07, SBI08]. **acetaldehyde** [Lu09, YLZ08, Lu09]. **Acetalization**
 [RUPH06]. **acetals** [MGG06]. **acetamide** [CCK01]. **acetate**
 [GWM08, PGG06]. **acetic** [MH08a, YT03]. **acetonitrile**
 [ELK⁺09, GJK00, NL07]. **acetylcholine** [GCD⁺08, MCK05].
acetylcholinesterase [MCK05]. **acetylcholinesterase-catalyzed** [MCK05].
acetylene [DLD⁺02]. **AcF** [GHLK⁺02]. **acid** [CJK⁺02, CMLS05, CJDK09,
 CCK01, DP03, DP04, DLHC06, DHW⁺07, FZL07, HFHL06, HLC09, IT03,
 IKYM09, JPF⁺00, JKM08, JCL05, KLB03, LL07, MT03, MMLC05, MSF⁺08,
 MH08a, Nak07, NHH05, NLL⁺09, Pac06, RR05, RKH03, SKGS00, SYC03,
 SL04, SBG09b, SWR06, SHK⁺05, UNHYT06, VM02, XSHC06, XLC08,
 XLT07, YT03, YXL⁺09, ZZY07, ZZY08, Z0J⁺06, vDSSvA04]. **acid-3**
 [vDSSvA04]. **acid-catalyzed** [RR05]. **acid-nucleotide** [MSF⁺08]. **acidity**
 [ELK⁺09]. **acids** [BE06, CADW03, CLA⁺00, FM00, HWTL03, HP04,
 IKYM09, KS01a, LDY⁺08, MB00, MM05, NHH05, OMNH08, PPYS08,
 Van02a, XKKL03, YLL⁺09, ZLD09]. **AcO** [GHLK⁺02]. **across**
 [HZX04, SSM08, SRB06]. **act** [GM01]. **actinide**
 [AB00, GHLK⁺02, NSO⁺07, VMA03]. **Activation**
 [EL06, BGC⁺09, BZL05, CC09, CFER04, KT08, Lu09, PV07, RRS06, Vya01].
active [AG00, BSDM04, CFR06, CFS⁺09, FCP⁺04a, FCP⁺05, HBM06,
 HFS⁺07, HYR06, JHPRSM⁺05, KSK00, KZRO03, LLL03, MDA08, PMM06,
 RZWS07, SS05, SFR07, TDH06, XLZ08]. **active-site** [SFR07]. **activities**
 [HMMS09, MS04, ZWB09]. **activity**
 [AGMPRG⁺08, Bou01, CW02, DD08, DA01, DHW⁺08, DHW⁺09, FTLV01,
 GDPP08, LC09, MRS09, Sha02, WZY04, Zer08]. **acylation** [MCK05, MK02].
adaptable [KF08]. **Adaptation** [HLM05]. **adapted**
 [FCP⁺04b, HdS06, HD06, LWX07, PTC01]. **Adaptive**
 [BHW00, HBW00, HBW01, HW03, HLSH05, DK01, GY08, OM04, RNG03,

SJJ⁺⁰⁴, WCS09, LS08c]. **addition** [BLO⁺⁰², DGD⁺⁰⁵, LL00, Mui05, RAGLL09b, RR05, WCW08, WSC09]. **addition-elimination** [Mui05]. **additions** [AVB00]. **Additive** [GGK⁺⁰⁸, CCK01, LKA01]. **adenine** [KKMMS04, SG07a]. **adenine-thymine** [KKMMS04]. **adenosine** [MRS⁺⁰⁷, YKK09]. **ADF** [tVBB⁺⁰¹]. **adiabatic** [SLRC01, TVL⁺⁰³]. **ADMA** [EM03b]. **admissible** [WG02]. **adrenergic** [YKK09]. **adsorbate** [BWI⁺⁰²]. **adsorbed** [DR09, PBZ00, XPW09]. **Adsorption** [ATH⁺⁰³, BRS00, BRS01, HSF08, ZTP⁺⁰⁸, NK06, SURG06, ST04, WLX⁺⁰⁵, ZCS04, ZSC05]. **Adun** [JGVF05]. **advanced** [LAEL01]. **advances** [MMRVH07]. **Advancing** [PP08b]. **affect** [AST06]. **affinities** [AVS09, DJ04, KS05a, KKMMS04, LLXS02, MRS⁺⁰⁷, SRB06, WSM⁺⁰⁸, ZJM⁺⁰⁷, ZXL⁺⁰⁴, dSGCG00]. **affinity** [ABA⁰⁴, FO08, GCD⁺⁰⁸, KFB05, KS08, Lee09, LXW⁺⁰⁹, MML⁺⁰⁶, RTG00, SOOF05, SWV⁺⁰⁵, ZWB09]. **affording** [OY01]. **after** [TJM⁺⁰³]. **Ag** [GPSP06, LYZ⁺⁰⁸, NA06, SG07a, WCS09]. **against** [SSS⁺⁰⁹]. **AGBNP** [GL04a]. **AgBr** [Sha02]. **agent** [LHJ⁺⁰⁶]. **agent-based** [LHJ⁺⁰⁶]. **aggregate** [KHF⁺⁰⁹]. **aggregates** [AB08]. **aggregation** [IM06, OGH05]. **AgN** [ZX08]. **agonists** [GCD⁺⁰⁸, SBG^{+09a}]. **Agreement** [LS05b]. **aided** [PJB⁺⁰⁷]. **AIM** [SFC04, CFS03, WW03]. **AIM2000** [Ano01a, BKS02]. **AIM2000-Program** [BKS02]. **Al** [OS08, WZZ⁺⁰⁹, Van08, KKJH08, QB05, WZZ⁺⁰⁹]. **al**. [RKH03]. **Ala** [PC00]. **alanine** [DSR⁺⁰⁷, ECA06, GAIMVB01, GSB09, GKTS04, HHP04, HMK02, JW06, LSW⁺⁰¹, MOP⁺⁰⁷, MFR07, PFJ⁺⁰³, Qua07, WD04, ZW09, ZM06]. **albicans** [RGP⁺⁰⁷]. **Alchemical** [Blo04]. **alcohol** [FBDG06, JJH01, KBN02]. **alcohol/water** [FBDG06]. **Alcohols** [ACLD03, LCDA03, LCGA03, LCA03]. **aldehydes** [LLA01d]. **Alder** [Hir08]. **algebra** [AT02]. **algebraic** [Tor02]. **Algorithm** [GGB07a, GGB07b, KSU03, MO01, WM12, ASWG07, AM06a, AM06b, AGSFAL05, BP02, BED02, BA08, BMTSC01, BSH07, BHH⁺⁰⁹, CS02, CLZX09, CWV⁺⁰⁵, CF04, DDKV07, DP03, DP04, DSR⁺⁰⁷, DBGV07, DAK08, FKFG08, FCP^{+04b}, GF08, GLD08, GCD04, GM04, Gon07, GKK07, HHJ03, HH04, HM06, HLM05, Ish04, IPN06, IPN07, JCA⁺⁰², KH01, KM00, KMA⁺⁰⁷, KUB07, KvGH01, KH06, LJZ⁺⁰⁷, LJS05, LM03, LMO09, MP03a, MP03b, MVLG06, MM07, Nak02, OR05, PV03, Rap06, RHL09, SKSH07, SJJ⁺⁰⁴, SWR06, SSMW09, Ste04, SBH02, TYO⁺⁰², TGD05, VGO⁺⁰⁷, WRBV03, WCS09, YK00, YGZZ05, ZBS03, ZZ08, ZA07, vLBBR12]. **Algorithms** [LMH⁺⁰⁹, BYQS03, BdPRMAI00, CKMC04, CSRST04, CHMI05, DB06, FS98, FS00a, HWDB03, KOFF09, OTL08, OGH05, RLER04a, SE08, TP01a, VW04, WK01, YL06, vLBBR12, HBW00, HBW01]. **alignment** [BA08, CLZ⁺⁰⁹, CLZX09, HHG⁺⁰⁹, RI07, VGDSU08, Leh06]. **alignment-free** [VGDSU08]. **aliphatic** [MSR04, SDvG01]. **alkali** [JHMB⁺⁰⁹, JHMB⁺¹¹, WWT08, ZWY⁺⁰⁹]. **alkalimetal** [BSG07]. **alkaline** [JHMB⁺⁰⁹, JHMB⁺¹¹]. **alkaloid** [BMRF01]. **alkane** [HGMB04]. **alkanes**

[BL09, VVBV02]. **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, ITN+05, IS07]. **all-purpose** [JGVF05]. **all-siliceous** [LST08, LTV08]. **allene** [WMRW+01, ZKZ+07]. **allenes** [WCHW09]. **allocation** [SKSH07]. **allosteric** [LGB+09]. **Allostery** [Sen06]. **alloys** [GD09, KGD06]. **allyl** [ZGZX07]. **AINC** [MLCD01]. **alpha** [GKK07]. **Alpha7** [GCD+08]. **AIPO** [PHH+08]. **altered** [DLRZ09]. **alternating** [YFR05]. **alternation** [JPCA08]. **aluminophosphate** [LMV07]. **aluminum** [TBG00]. **always** [Kol04]. **Alzheimer** [MS03]. **AM1** [DC02, FRS05, JBB00, JJB02, LMMW04, RFSS06, TCT03, VGGMM05]. **AM1-BCC** [JBB00, JJB02]. **AMBER** [Ano06c, WWC+05, CCD+05, FSFK05, JS07b, JM07b, MRC03, OYH05, TdMSD+08, WCC08, WWC+04, WZW+06, WS07]. **AMBER*C** [CLA+00]. **AMBER95** [ONHN00]. **ambiguous** [BS01]. **Amica** [GBL+05]. **amidase** [CBS+03]. **amide** [CCK01, GSB09, LKA01, SJW09, YSA+03, IINK09]. **Amide-** [IINK09]. **amides** [CMLS05, KS06]. **amine** [OY03, PS03]. **amines** [CLFA07]. **amino** [CADW03, CJDK09, CLA+00, DLHC06, DHW+07, FDSA00, HFHL06, HLC09, IT03, IKYM09, JPF+00, KS01a, KLB03, LDY+08, LL07, MT03, MM05, MSF+08, NLL+09, RKH03, SURG06, SKGS00, VM02, XSHC06, XLC08, XLT07, XKG+05, YLL+09, YXL+09, ZLD09, ZOJ+06]. **amino-cyclopentene** [SURG06]. **aminoarabinonucleosides** [BL08]. **Aminopurine** [SC01]. **aminoribonucleosides** [BL08]. **aminosubstituted** [TKS+01]. **ammonia** [HT05]. **ammonolysis** [UNM+01]. **among** [IGNH03, LLL07, WS07]. **amorphous** [CA04, CA07a, CA07b, SHH07]. **AMP** [FKM+06, FKM+07]. **amplitude** [KS05b]. **Amyloid** [BTP09, MS03]. **amyloidogenic** [CP09]. **amylose** [NK01]. **anabolic** [AGMPRG+08]. **analgesic** [CMBC08]. **analogs** [AS09, BWE05, FPG+06, FKJ+01, HFHL06, LFEeL06, MT03, VM02]. **analogue** [LRI+02, WC08]. **analogues** [BISB02, WHP02, XYN+06, ZSE08]. **analyses** [BLT03, CZ05, DRAS05, HN02, Hir08, 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, CCP04, CSRST04, CA07b, DDKV07, DRAS04, DSR+07, ECM+03, FK07a, FC06, FSS00, Gly06, GS07, Gra07, GHBB04, HHWG08, HS00, HLSH05, HP05, IN08, JPF+00, JMD+02, JFG04, KB02, KK08a, KMH02, KSU03, KN04, KSK00, KMA+07, Kni00, LRI+02, LS05a, MGCA07, MS03, MWE02, MHW04, MMP+07, MA05, NK06, NSU+02, OML+00, ON07, PFC03, PGH+04, PP08b, PYEA03, PAS07, PYCD03, PYS05, PC07, PLC08, RMHK03, RS07b, SH09, SMGE08, SSHT03, SFC04, SCF+09, SvDS01, TYN05, TCR+02, TT01, TD06, TTB01a, TTB01b, UTH+03, VGB08, VKCK09, WRBV03, YNW05, YK08, ZSE08, Zer08, ZWB09, ZHH09, ZB07, NYK+09, Ruv07, VB09, RS07a, VB07]. **analytic**

[ASWG07, DOSG06, GL04a, IK00, KBT03, LFSB03a, LFSB03b, SJW09].
Analytical [HNWF07, HNWF12, PDC⁺08, QCK01, QCK02, RLR⁺04, WL02, DSR⁺07, HC08, HHS⁺05]. **analyze** [AGMPRG⁺08, Ham07, MCF07].
analyzing [DW08, LD05b]. **andradite** [ZWTP⁺08]. **anesthetics** [TZX01b, TZX01a]. **AnF** [Han01]. **Anglada** [Bof01, Qua01]. **angle** [CIB05, FWH⁺07, LI07, OFIK09, YL06]. **angles** [FPG⁺06, FKZ09, HK08c, WHRG08]. **angular** [GY08]. **anharmonic** [BP07, DB07, GBDP05, LMO09]. **anilido** [GTC06]. **anilido-imine** [GTC06].
Anion [JT06, CW02, DMN05, EFQD09, GS04, wQZsLyZ02, QZZZ03, VDM06, WLZ⁺07]. **anion-** [EFQD09]. **anionic** [ALC08, HHWG08, PGG06].
anions [CTFC08, KKMMS04, Lee09, LLXS02, Owe05, ZXL⁺04].
anisotropic [BCIB05]. **anisotropy** [GKTS04]. **ANN** [HSMT04]. **annealing** [ADM⁺06, CS02, CCP04, HPP00, KH01, LCKL05, LJKL08, MCF05, WG02].
annexin [MHJS06]. **Announcements** [Ano05a].
annulation [GLH⁺08]. **anomeric** [CPJ00, CPJ01, CKF01, LCDA03, VM07].
ant [CLZ⁺09, CLZX09, DDKV07]. **antara** [LFS⁺07]. **antara-antara** [LFS⁺07]. **anthracene** [CG08, CDPL09, HIA03]. **anthracene-9** [CG08].
antibacterial [YCW⁺09]. **antibody** [CBS⁺03, SOOF05, TH02, UTH⁺03].
antibody-catalyzed [TH02]. **anticancer** [BZL05, PFR04a, SMM⁺08].
antifungals [GDPP08]. **antigenic** [WCF04]. **antiinflammatory** [CMBC08].
antilipid [MRS09]. **antimicrobials** [GDPP08]. **antitumor** [KC01a, WM01].
apatite [RD06]. **Applicability** [DC02, PRS04, QTdG⁺08]. **applicable** [PB05]. **Application** [ASDP⁺06, CIB05, DSR⁺07, GWS⁺02, HKMS01, HSMT04, HM08, HMMS09, KSS08, KAK⁺09, KBK⁺01, Mat03, MW09, TBSM09, TKN⁺08, BLN01, COS01, CSJ01, DLWV07, DV02, FOK⁺04, FKU⁺05, GLD08, GWM⁺00, HHH00, JW06, JGVF05, KTM02, KK01a, LL00, LFSB03a, LFSB03b, LI07, LSHR04, LCSZ09, LXL07, LLL03, LMO09, MG00, MS04, PB04, RI07, Rud05a, SG07b, Tot04, VM00, Wil01b, WR07, ZLY07, ZNLL07, dGWH01, CMJ08, CWV⁺05, CMBC08, GRO⁺03, GBDP05, GS04, IN08, IS03, LJZ⁺07, LSY02, MB00, MCF05, MBC08, MTB09, ON07, PHJ⁺08, Qua04, QCK01, QCK02, Rud05b, Rud05c, SL09, SDCG02, SFC04, TH02, VVS07, VKCK09, WRP⁺06, WFR08, vGGB00]. **Applications** [HLLN06, BWZ08, BBG⁺04, CGMPT⁺08, CR09b, Est07, LW06, PMC⁺08, PTC01, SPF⁺07, Tor02, ECM⁺03, GGB07b, HT03, RSN⁺02, WNH03].
applied [ADM⁺06, BL09, BT00, BS06, DMN03, FII⁺07, GHK⁺02, MKGA06, OM04, TLKT00, YAÇ⁺02, ZZ08, dVB01, BBC⁺05]. **Applying** [AGMPRG⁺08, Woo01, You11, GS02]. **appreciation** [vRS01]. **approach** [AB00, AGK03, AVS09, BG03, BME05, BS03, BGJ01a, BLF02, BMTSC01, BPCD07, CCWH02, CYM02, CGBF05, CAGR08, CMCB08, CG05, EM03b, GAIMVB01, GAI06, GJL⁺08, GRO⁺03, GDV03, GS02, GDPP08, GdSuM⁺07, GdAcV⁺07, GCD⁺08, HMMS09, Hin00, HRR05, HT03, HLSH05, IT03, KKG⁺09, KN04, KHY00, KHF⁺09, KBT03, LFKL00, LCC09, LMJ02, LYS08, LD05b, LWZ09, MAF⁺07, MR04, MFR07, Mor02, NYTH09, Oos09, PS09a, SAM06, SPGS08, SGPS09, SL04, SWZS04, VW03, Van02b, WWL⁺09,

XWC09, XKKL03, YS00, YK08, ZCS04, ZS04]. **Approached** [LL07, XSHC06]. **approaches** [BP07, Con02, CSD05, COL⁺06, MLJ03, PSF⁺08, PMM05, RLDI09, RSS09, SM08a, YCW⁺09]. **appropriate** [Bac07]. **approximate** [Cul08, 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, RP07d, SHSF05, ZFL⁺05]. **approximations** [Dya02]. **APS** [CBC⁺08]. **APX** [ZJM⁺07]. **aqua** [RMP01]. **aqua-** [RMP01]. **aqueous** [BISB02, CPJ00, CPJ01, CW02, CCK01, DA01, EK06, FHRR07, HMWC03, HRR05, HDO⁺02, IV04, IvSV06, JM07b, KEH⁺02, KPR04, Kri08, Kri09b, LRI⁺02, LR03b, Loe03, LMIF06, MM02, NL07, PK04, PHRR08, SH09, SMKMO0, SBB02, VP09]. **arabinonate** [RGP⁺07]. **arabinohydroxamate** [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** [FKŠ⁺09, PCMG09, RRZA08]. **arene-containing** [RRZA08]. **arginine** [ČJPZS08, SMGE08]. **arginine-bound** [ČJPZS08]. **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-Backbone** [CPML08b, Van08, PCO⁺07b, PCO⁺07a]. **aromatic-type** [HLC09]. **Aromaticity** [BPCD07, FMPS08, JHMB⁺09, JHMB⁺11, LWW⁺06, LTF⁺07, MGMM07b]. **Array** [FJP07, ABF⁺03]. **arsenic** [ALC08, KS05a, ZXL⁺04]. **ARTE** [VB07]. **ARTE-QSAR** [VB07]. **artifacts** [CCSJ00]. **Artificial** [PS09a, RWBH09, dVB01, CLC03, Gol09, NINAT⁺07, TCSM03]. **arylamide** [VIP⁺06]. **ascorbate** [HBM06]. **ASIC** [NYTH09]. **aspartic** [ZZY08]. **Aspects** [HHBH00, MO01, BMRDB01, BRS07, Sie01, TT02]. **assemblies** [DFGB09]. **assembly** [DPRR05]. **Assessing** [IB04, FGR07]. **Assessment** [BP03, CCWH02, DGI⁺08, KS08, LWH06, SSS⁺09, WSM⁺08, CKMC04, FMPS08, GT03, LLS03, SP05, GGT08, GHBB04, TFZRG01]. **assignment** [BB05, BMRF01, PRJ02]. **assignments** [PF06]. **assisted** [BA04b, KT08, WJX⁺08]. **assists** [BM07]. **associated** [SWR06, TT08]. **Associative** [ABYM08, NL08]. **asymmetric** [WR07, WFR08]. **Asynchronous** [GLP08]. **atmospheric** [GCCVB00, PGNG03]. **Atom** [RP07a, RM00, BPC01, BR04, BWW⁺08, CCK01, FM00, GWS⁺02, GB04, HLLS05, IT03, JS07a, mJIZyL⁺08, LMK01, MT03, MB00, PHH⁺08, RG08, RS08, SSB⁺03, SBLK01, SLL⁺04a, TGLL07, VK06, VGO⁺07, WLL07a, WBSR03, WS07, WLL⁺03, YLWL09]. **atom-bond** [VK06]. **atom-centered** [SSB⁺03]. **Atomic** [DVP⁺02, FDM00, AS00, Bac07, BSC⁺01, BCNs07, BSP06b, BK00, BLT03, BAÅ07, CN03, FS04, GC02, Ish03, JBJB00, JJB02, KRM⁺02, Kau07, KS01a, KC01b, Lab08, LMV07, LST08, LTV08, Nil09,

PGG06, PSMB05, RKA⁺⁰⁹, SvDS01, TBSM09, UBDPJ04, VZVG06, VC04, XLT07, YOB⁺⁰⁸, dSGCG00, DVRP⁺⁰³. **atomic-centered** [TBSM09]. **atomistic** [CA04, IDMC09, KK01b, RPMP03, SPGS08, ZALMG03]. **Atoms** [VM07, YK08, ALTB06, AD00, ASS⁺⁰², BHTCG07, BKS02, BS03, CMJ08, CDS09, EdIVR⁺⁰³, FS04, HSF08, mJlZsLyL07, 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** [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** [JČHS07, 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, SMAAdv00]. **averages** [Rap06]. **averaging** [BSC⁺⁰¹]. **avian** [DLRZ09]. **avoidance** [WCFH02]. **axial** [BMRF01, CN05]. **axis** [OMNH08]. **azaglycine** [LKJ⁺⁰⁴]. **azide** [MSR04]. **azides** [ZX08]. **azido** [PFR04b]. **azole** [SMM⁺⁰⁸]. **azole-bridged** [SMM⁺⁰⁸]. **azurin** [PMGL03].

B [OS08, Sta00, WZZ⁺⁰⁹, WD08, ZZZ⁺⁰⁶, ALKH04, BAL⁺⁰¹, FH01, GL04b, JS07a, KVS⁺⁰⁶, LMGR06, 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, CLWL09, HSWN01, KLS02, LKA01, MFB04, MLL08a, PCO^{+07b}, SP05, WZW⁺⁰⁶, YL06, PCO^{+07a}]. **backward** [KM07]. **bacterial** [Ano06b, CPM03, GS04]. **bacteriochlorophylls** [LKT04]. **bacteriopheophytin** [IN01]. **bacteriorhodopsin** [RG02]. **Bacteroides** [SDM02]. **Bader** [GHBB04, SKSH07]. **Baker** [WB05]. **balance** [Ano06c, WZW⁺⁰⁶]. **balanced** [PB05]. **Balancing** [CF06]. **band** [AJ03, JCA⁺⁰², ZZW09]. **Baoshan** [JW12]. **bare** [KT08]. **barrier** [CRGN07, KSTC01, LSG06, MG06]. **barriers** [DBM03, EL06, HFHL06, PBF09]. **bars** [MDI04]. **base** [CCK01, DP04, FZL07, HWTL03, KKMMS04, MMLC05, MSF⁺⁰⁸, MHS05, NL08, OY01, PG04, PSS⁺⁰⁴, PSMB05, SKGS00, SG07a, ŠBL05, SC01, SYC03]. **base-catalyzed** [OY01]. **base-pairing** [DP04]. **based** [Adc04, ALTB06, ALB09, AB09, BdPRMAI00, BMRF01, BDW00, BMTSC01, CGMPT⁺⁰⁸, CKR08, CLZ⁺⁰⁹, CLZX09, CFK08, CHA⁺⁰⁷, CPUGD09,

CMBC08, CRGN07, CA04, CSB⁺⁰³, DLW06, DMLI05, DHW⁺⁰⁰, DB02, DDVD09, DHW⁺⁰⁷, DHW⁺⁰⁹, DWC⁺⁰³, FCK⁺⁰⁸, FCP^{+04a}, FCP⁺⁰⁵, FM00, FZL⁺⁰⁶, FRLN09, GZL02, GRCD01, Gon07, GDPCPU07, GDPP08, Gra07, GAS04, HSMT04, HS07b, HLM05, HZ06a, HZ06b, HMOG07, IIK09, IR03, JD09, JKII08, JGVF05, KLS02, KBA⁺⁰⁴, KK08c, KBK⁺⁰¹, Kob03, KIM⁺⁰⁹, KZW⁺⁰⁵, KVS⁺⁰⁶, LFKL00, LHJ⁺⁰⁶, Leh06, LXZ06, LJZ⁺⁰⁷, LH05, LLM09, LM03, MLL06, MSF⁺⁰⁸, MSH^{+06a}, MBH⁺⁰², NLL⁺⁰⁹, NMAT01, OVMV04, PS09a, PFR04b, PA05, PAS07, PRJ02, PF06, PRDS08, Pul05, QLHL09, Rao00b, RSE07, RSER09, RLDI09, RSN⁺⁰², RKA⁺⁰⁹, RUPH06, RRS09, RSS09, Ruv07, SAM06, SKSH07, SGPS09, SPL⁺⁰², SBB02, SE08]. **based** [SZW⁺⁰⁵, TTBM09, Tot04, VSK⁺⁰⁴, VB09, VGDSU08, WL09a, WL00, WS07, WRBV03, XYN⁺⁰⁶, XL02, YWHZ03, YNW05, hYDN⁺⁰⁸, YJF06, YXL⁺⁰⁹, YKK09, ZCL09, ZLY07, ZLD09, ZWB09, dSR08]. **basepair** [BCP03]. **bases** [CCK01, Nak07, RTG00, RKH03, SL04, WRP⁺⁰⁶]. **basic** [Rud05a]. **basicity** [EK06, Lee09]. **basins** [CFS03, MP03a]. **Basis** [AHK02, BRLS08, BRLS12, JJK⁺⁰⁰, Wib04, ABF⁺⁰³, ALKH04, Bac07, BY06, BR04, BT00, BSOB05, BRV⁺⁰⁷, CMJ08, CRS05, Cul04, CGSdST06, DMZT08, EA08, EdIVR⁺⁰³, EL09, FZL07, GKH05, HdMdS05, HdS06, HD06, IO08, JSHG07, KK08a, LFK05, Lai07, LMV07, LST08, LTV08, MV06, Mas04, MLL^{+08b}, MC06, MY08b, MY08a, NSO⁺⁰⁷, OBBS05, PSC⁺⁰¹, Pen06, PFJ⁺⁰³, PSMB05, RRP⁺⁰¹, RLRE01, RLER07, SSB⁺⁰³, SNM⁺⁰⁶, TSSSG08, VKP⁺⁰⁸, VB03, Var09, VKCK09, WMGK07, WTKM06, Wei08, ZWPR⁺⁰⁴]. **Basis-set** [AHK02, MV06, Pen06, VKCK09]. **BCC** [JBJB00, JJB02]. **be** [HdMdS05, HdS06, HD06, IGL07, STSF02, WCF04, BP01, LWW⁺⁰⁶]. **beam** [BAL⁺⁰¹]. **bearing** [NL08]. **Becke** [AAP00]. **Becke-3** [AAP00]. **Becke3** [PDS01]. **Becke3-LYP** [PDS01]. **BeH** [PRSMV08]. **behave** [PB02]. **behavior** [Ama02b, Bac05, BISB02, LB05, OO04, RP07c, SBI08]. **behaviors** [LML⁺⁰⁰]. **being** [OCB02]. **benchmark** [Ano01b, BSB05, DGD⁺⁰⁵]. **Benchmarking** [Hol05, SZT08, WS07]. **Bennett** [KBB09]. **Benzdiynes** [ASY01]. **benzene** [BE09, BRLS08, BRLS12, HT05, HRG07, IINK09, LWX07, Sch00, SG07b, ZTP⁺⁰⁸]. **benzenes** [PB05, WRP⁺⁰⁶]. **benzo** [GLRL02]. **benzocryptand** [WWT08]. **benzodiazepinone** [SPGS08]. **benzodioxoles** [MRS09]. **benzoic** [BE06]. **benzonitrile** [ZH08]. **benzylideneaniline** [BY06]. **benzylpenicillin** [DSS03]. **Beowulf** [BMRDB01]. **Bergman** [PWFS01]. **Besalú** [Bof01, Qua01]. **Bessel** [DBS08]. **Beta** [LHI09, BTP09]. **Beta-hairpin** [LHI09]. **between** [AD00, AZM03, BS03, CFR06, DRAS05, EFQD09, FG03, FL07, FO08, FKM⁺⁰⁶, FKM⁺⁰⁷, GWM08, HPP00, HRBKB03, HFHL06, HN02, Hir08, IINK09, JPCA08, KWK⁺⁰¹, KWK⁺⁰², LDC⁺⁰⁷, Li01, LL01, LFZS04, LLL03, LS05b, MST⁺⁰⁸, MBH⁺⁰², OY01, PSF⁺⁰⁸, PMPGP05, PS03, RLRE01, SM08a, SBLK01, Sim07, SWM04, SKK⁺⁰⁷, SP05, TYN05, TK08, TDH06, UTM⁺⁰², UTT⁺⁰⁴, WLX⁺⁰⁵, YT03, YQQH09, Yos02, ZZTS09]. **beyond** [CLP⁺⁰⁵, CCK01, Haf08, PP08b]. **BH** [QZL⁺⁰⁴, SAS05]. **Bi** [LS08a, WL09b, HZ09]. **bi-transition** [WL09b]. **bias** [OM04, SY09]. **Biased**

[MLG04, KV00]. **bicyclic** [EBDPM00]. **bicyclo** [BE07, BPC01]. **bifurcation** [CPFL02]. **bilayer** [CEP07, HNL08, MCR08]. **bilayers** [JM07b, RG08]. **bimetallic** [WCS09]. **bimolecular** [ML00]. **binary** [Kle02, Kle03, LCSZ09].

Binding

[ABÅ04, AGO⁺02, BCP03, RGP⁺07, ABYM08, AM06b, APG05, AVS09, BWE05, BSP06b, DLRZ09, Dra00, ECM⁺03, FKU⁺05, GCD⁺08, GS04, HT05, HNWF07, HNWF12, IO08, JMD⁺02, JZD⁺09, KFB05, KS08, LXW⁺09, MK02, MHJS06, MLL⁺08b, MRS⁺07, NyHN06, NHN06, OYH09, OFIK09, PMGL03, RSP03, RGG08, RK05, Ruv07, SOOF05, STSF02, SWV⁺05, TGGP⁺00, VGGMM05, WM04, WHF08, Wou00, XL02, ZGFL01, ZWB09, KEB04].

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

bioinorganic [MSH⁺06b, SGD06]. **bioisosterism** [DPM09]. **biological** [CCK01, CMGDAC⁺07, GdAcV⁺07, HMMS09, LDTS07, Mac04, TH02, WCK00, YPNE09, 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, LSO04, OVMV04, WB04a, WB04b, WB05, WL09a, ZFW08].

biomolecule [ABWT09]. **biomolecules** [ECM⁺03, Est07, FEVM01, HMD06, KHY00, MMLC05, QSS01, YNZ⁺08, YJF06]. **bionanosystem** [MO09]. **biophysical** [Mat03]. **BiOX** [HZ09, Hua09a]. **biphenyl** [PCMG09].

biradicals [KC01a]. **bis** [BLN01, CDL06, PYS05]. **bis-heteropentalenes** [CDL06]. **bishomoaromaticity** [HWGB01]. **bisphosphatase** [MRS⁺07].

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

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

Blue-shifting [HRG07]. **BLYP** [TCT03]. **board** [ATMK03, KAK⁺09]. **boat** [RP09]. **bodies** [FS98, FS00a]. **body**

[CCK01, FII⁺07, FBDG06, Ike04, Loe03, SM03, TKH07, LR03b]. **Bofill** [Qua01]. **Boltzmann** [WB04a, WB05, ABWT09, BHW00, BBP09, BH03, BF04, BF07, GPN01, GCD⁺08, GGT08, Höf05, HBW00, HBW01, KWHH07, LDG02, NYTH09, PZS04, SATO04, VZM⁺08, WB04b]. **Bond**

[CGMPT⁺08, CRC⁺08, JG03, MGCA07, May07, SH08, WM12, Bic09, BL06, CMLS05, CPFL02, CPDZH08, CJW⁺09, Cul08, DR09, DGD⁺05, DMZT08, FH01, FO08, GYMN07, GR07, GS07, HRG07, HS07a, Hir08, JPCA08, JP09, Kle03, KBLP09, LC07, LZC09, LS08c, LS05b, MG00, OO04, Pac06, PSC⁺01, PAS07, PYS05, PV07, Rao00a, RM07, RCJ02a, RD00, SEKS09, Sha07, Sim07, SPT⁺03, SWZS04, SMZW05, SSMW09, ST01, SSW⁺07, TJM⁺03, Tru07, VK06, VBGL⁺00, WHRG08, WJ00, XWXC08, vLBBR12].

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

[CPDZH08, Gon07, HT03, IO08, LB05, LDL⁺09, LZF⁺09, McD08, MH08a, NBTN04a, NBTN04b, NL08, PHFC04, ZH08, vEMK01, vE01]. **bonding**

[AM07, AG00, Bac04, Bac05, Bac07, BHTCG07, BM07, BSG07, CWWS07, CQ04, CCK01, EFQD09, FLK⁺07, FK07b, Jac09, Kau07, KJP⁺07, KBL08, Kle02, Kle03, KGD06, LW07, LWK08, LDL⁺09, PG01, PYCD03, PLC08, RPNJ07, RP04, RS07a, RS07b, SM08a, SG07a, SCP08, Wil01a, WD08, WWS07, XZ04, XK08, Yos02, ZX04, ZW09, ZB07]. **bonds** [Bac05, BUMCMRL00, BRS07, CRC⁺08, DR07, HA04, Mit01, NHH05, OO08, PGG06, 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** [ČJPZS08, WC09]. **Boundary** [BH03, ABWT09, Ara04, BVW04, BF04, BF07, HH04, KWHH07, QSS01, TK08, WM06]. **bovine** [MBC08]. **bowls** [LMGR06]. **box** [LM03, WM06]. **box-counting-based** [LM03]. **boxes** [MBP09]. **Boyd** [Sta00]. **Br** [FHF⁺01, HZ09, Hua09a, KBL08, Mar03, RB01, STC⁺08, WLLS04, ZJM⁺07, ZY01, ZL09b, HYA02, LDC⁺07, RFSS06, SLL⁺04b, WLLS05, ZZW⁺07]. **brain** [CRGN07, HMSM06]. **BrCl** [WLLS05]. **breakage** [SWR06]. **breakage/closure** [SWR06]. **breaking** [HRR05, Pac06, VHRR07b]. **breast** [VGDSU08]. **Breit** [Ish03]. **bridge** [CFC⁺08, PAS07]. **bridged** [LHP01, SMM⁺08]. **bridges** [KF03]. **broadly** [PB05]. **broken** [ATH⁺03, BB08]. **bromine** [WyLG⁺09]. **bromine-substituted** [WyLG⁺09]. **BSSE** [GAI06, PSC⁺01, SPDS01, SAM06]. **BSSE-corrected** [PSC⁺01]. **BSSE-free** [SAM06]. **Buckminsterfullerene** [NRKH02]. **buckycatcher** [Won09]. **Buff** [KS06]. **build** [BMTSC01]. **build-up** [BMTSC01]. **Building** [BCIB05, BAÅ07, GKK07, HP05, MABM09, PC00, PFC03, Fau01]. **built** [GFS05]. **bulk** [BACJCT01, BGC⁺09, EBL⁺08, JBGK08, LZCC09, LLL03, PB04]. **bulk-doping** [JBGK08]. **butadiene** [GRO⁺03, Hir08, WR07]. **butanal** [NSB08]. **butanes** [WW04]. **butyl** [Bac09].

C [Ano00, BAL⁺01, BPC01, BSB05, Bic09, CTFC08, HK07, mJIZyL⁺08, KYFW07, KJP⁺07, KSN01, LYZ⁺08, Mck07a, Mck07b, Owe05, SLL⁺04b, VBS09, WLL01, WDXS06, WZZ⁺09, XFF06, YHD⁺06, ATBLS04, Ber03, CPDZH08, CCB04, CS01, CRSB03, CTFC08, DGD⁺05, DRAS04, Eli07, FHF⁺01, GYCZ04, GZ07, GB02, HBM06, HYA02, HK07, HA04, IN08, LDMR01, LMK01, Mit01, OO04, PRSMM03, PV07, RD00, RFSS06, SLL⁺04b, STC⁺08, TYN05, WLPF05, WDWS06, Wil01b, XDS06a, XWXC08, ZZL04, ZW09, ZLD09, ZZvRSC08, dRLMS00]. **C-PCM** [CRSB03]. **C12A** [BRDC02]. **C12A-p8** [BRDC02]. **C96** [ONHN00]. **Ca** [WZZ⁺09, WD08, XWC09, HLB09, 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, RSSKB03, RM00, Wib04, WM04, ZXY08, Kle03]. **calculates** [ATMK03]. **Calculating** [Chu07, CG05, DRMD03, DF04, LN01, MC06, PDC⁺08, PMM05, RSE07, SYC03, WCK00]. **Calculation** [BK00, CPML08a, DJ04, KKY01, KRM⁺02, LSW⁺01, MT03, MO01, MRS⁺07, TS05, VM02, VC04, WKYU01, ZWPR⁺04, BP02, BSC⁺01, BH03, ECA06, FOL⁺04, FROD08, GKRG08, GLMV09, GAdGM08, GGT08, HTKG08, II02, ITN⁺05, JJK⁺00, KFNH08, LFK05, Li01, LLZL09, MGLO03, NRKH02, Nil09, OCP02, PZWG⁺04, PRSMV08, RNG03, Rap06, RLER04a, RKA⁺09, RRFC⁺03, SOOF05, SKGS00, STSF02, SSM08, SHH07, TZX01b, TZX01a, TLOG00, TP01b, TRS02, TKN⁺08, UKN04, UIHN09, WLLS05, WLL⁺07b, WSM⁺08, WM01, XOW⁺00, ZWB09, ZL09b]. **Calculations** [YH07, Ano01b, ALKH04, Bac09, BP07, BSOB05, BMRDB01, Blo04, BMB07, BMRF01, BWI⁺02, CLP09, CMJ08, CN03, CRS05, Chi03, CS03, CMA⁺08, DB07, DPDG05, DSS03, DMJV05, DWC⁺03, EKO⁺01, EBL⁺08, EL09, FKFG08, FL08, FMSA06, FR06, FO04, GJL⁺08, GBDP05, GM04, GWM⁺00, GBB07, GPSP06, HHH00, HLLN06, HYA02, HMSM06, HFHL06, HKHN08, HT03, HWGB01, HZ09, Hua09a, Hua09b, ILKR09, IGL07, IPN06, IPN07, JCA⁺02, JBGK08, JČHS07, KGL07, KWHH07, KRLD09, KTM02, Kob03, KBLP09, KS02b, KKS04, LLA01a, LLA01b, LLA01c, LLA01d, LLA03, LFSB03b, LDC⁺07, LHI09, LWH06, LC06, LKW04, LZF⁺09, LS05b, LDG02, LMO09, MMLC05, Maz08, MBL⁺00, MA05, MLCD01, MLJ03, MS01, Mui05, NYK⁺09, NTH09, NSU⁺02, OBBS05, OYH05, OS06, OKH⁺02, Oos09, OKE⁺02, PB06, PMGL03, PVdJB00, PV03]. **calculations** [PBZ00, PRSMM02, PSS⁺04, PSMB05, RSP03, RMP01, RP02, RRCA08, ROG00, RWBH09, RS05, RRS07, RJLR06, SBI08, SSB⁺03, SCS07, SBG⁺09a, SHM04, Sha02, SSL02, SN06, SFRS01, SMG09, SG01, TK08, TY03, UKNS01, UTM⁺02, VKP⁺08, VZVG06, Van02b, VE09, VIP⁺06, WL02, WTKM06, Whe08, WC04, WHF08, WR07, WFR08, WHG⁺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, IGL07, Mck07a, WCF04]. **cancer** [VGDSU08]. **Candida** [RGP⁺07]. **candidate** [SF07]. **canonical** [BP02, EMP07, ITN⁺05, IS07, KM00, Kni00]. **CAOs** [PS03]. **capabilities** [GCD04]. **capped** [CZ05]. **caps** [ZCZ03]. **capsid** [KCL06]. **captopril** [AGO⁺02, APG05]. **capture** [YXC⁺07]. **Car** [JP09, Sch04]. **carbapenem** [BBSS06]. **carbazole** [YFR05]. **carbenes** [HA04]. **Carbohydrate** [KBN02]. **carbohydrates** [ACLD03, HR08, KDSV02, LR03a, LCDA03, LCGA03, LCA03, LH05, MW00, Sto05, KYT⁺08]. **Carbon** [KK08c, LMGR05, BSB05, BG07, CZ05, CDPL09, DWS⁺09, GKK07, HT05, KT08, KLS02, KK01b, LMK01, MMRVH07, PAS07, wQZsLyZ02, SRS07,

Wan09, WSC09, XWL⁺09, ZKZ⁺07, ZWY⁺09, ZZvRSC08]. **carbon-**
[ZWY⁺09]. **carbon-centered** [WSC09]. **carbon-rich** [CZ05]. **carbonate**
[vDSSvA04]. **Carbonyl**
[RD00, DLR⁺08, LL00, LLA01a, LLA01b, LLA01c, LLA01d, LLA03].
carbonyls [BRV⁺07, LMGR05, PLC08]. **carboplatin** [WM01]. **carboranes**
[JRJ01, OSA06]. **carboxybenzisoxazole** [UTH⁺03]. **carboxylates**
[ČJPZS08]. **CarC** [BBSS06]. **carcinogenic** [EL06]. **carcinogenicity** [VS08].
Carlo [AGSFAL05, AGSFA⁺05, BR03, BHG03, Der00, FCK⁺08, FKFG08,
GHH07, HMD06, IM06, IKYM09, KLS02, KM07, KKC05, LML⁺00, LZA02,
LRWG03, MH09, Nak02, NA06, NCO⁺05, OM04, SKGS00, SCS07, SBJ08,
SM08b, SWR06, TS05, XKG⁺05, ZCS04]. **Carlo-with-Minimization**
[NCO⁺05]. **carma** [Gly06]. **carrying** [Tor02]. **Cartesian** [LPK07, PHR⁺05].
CAS [PRSM03, BMB07, JHPRSM⁺05, PRSM02]. **CAS-SCF**
[JHPRSM⁺05]. **CAS-SDCI** [BMB07, PRSM02]. **case** [AB00, AS00,
BUMCMRL00, BWW⁺08, BS06, CFS⁺08, ČJPZS08, MV06, MDI04, Pac06,
PGG06, PC00, Pog03, RUPH06, SBI08, SN06, Van02a, WRBV03]. **cases**
[BCF⁺09]. **CASPT** [PO03]. **CASPT2** [KRLD09, WLZ⁺07]. **CASSCF**
[Bac04, Bac07, DOSG06, WLZ⁺07, dSVA⁺09]. **CASSCF/CASPT2**
[WLZ⁺07]. **Catalysis**
[UTH⁺03, DWS⁺09, QZZZ03, TH02, VBGL⁺00, ZDS⁺05]. **catalyst**
[VBGL⁺00]. **catalysts** [YXC⁺07]. **catalytic**
[CGB⁺09, KSK00, LS08b, MS04, NTH00, RWBH09, SPT⁺03, WC08, ZAT07].
catalyzed [AST06, BTP09, GVATG03, GLH⁺08, HSWW00, MCK05, OY01,
PHKG07, RR05, Sie01, TH02, TGLL07, WCW08, WCHW09, ZWS⁺09].
catastrophe [PA05]. **cathepsin** [ZWB09]. **cation** [DSB⁺02, Don08, LB08,
OO04, PV07, QZL⁺04, SLRC01, VL00, WLZ⁺07, WSM⁺08, Wou00, ZL05].
cation-water [DSB⁺02]. **Cationic** [JRJ01, TBG00]. **cations**
[ALC08, GSB09, GS04, GWL07, HIA03, Hol05, NSB08, RRS06, SZT08,
WWT08, ZWY⁺09]. **caused** [LPK07, TT08]. **cavities**
[BCIB05, BHH⁺09, IME02]. **cavity** [RRZA08, ZFL⁺05]. **C** — [CJW⁺09].
CBr [FHF⁺01]. **CBS** [Lu09]. **cc** [Wib04, GYMN07]. **cc-pVTZ** [WD04].
CCH [ZKZ⁺07, ZKZ⁺07]. **CCl** [ZLLS06a, FHF⁺01, WDZS07]. **cclib**
[OTL08]. **CCN** [JDWS06]. **CCSD** [BBI⁺09, Lu09, PFJ⁺03, PV03]. **Cd**
[GSP06, XB08, BMRF01, BBI⁺09]. **CD38** [UNHYT06]. **CDOCKER**
[WRBV03]. **Ce** [SNM⁺06]. **Ceccarelli** [Ano06b]. **cell**
[Gon07, KVS⁺06, KS05c, LEV⁺09]. **cell-based** [Gon07]. **cells** [CCCJ09].
cellular [XWC09]. **CeN** [VP08]. **centauric** [PA05]. **center** [BRS07, GGA00,
IN01, Lai07, MGMM07a, MGMM07b, NR04, OON01, SGPS09, TBG00].
centered [CCK01, SSB⁺03, TBSM09, WSC09]. **centers** [GYMN07, JKL08].
central [CGMPT⁺08, CM09]. **CeO** [CCCJ09]. **ceramic** [HZX04]. **cesium**
[HD06]. **CF** [mJIZsLyL07, YLWL09, LDC⁺07, gThDjL⁺01, UTM⁺02,
UTT⁺04, WLL⁺07b, YLW⁺08, YLWL09]. **CFCl** [mJIZsLyL07]. **CFF91**
[TTB01a]. **CFMC** [NCO⁺05]. **CH**
[CPJ00, GBDP05, HTN03, IN08, mJIZyL⁺08, LW04a, LDT⁺02b, MGLL03,

Mui05, RD00, SLL^{+04a}, TJM⁺⁰³, WLL07a, WLL^{+07b}, WDX⁺⁰², YLW⁺⁰⁸, ZZL04, ZZW⁺⁰⁷, ZZL⁺⁰⁸, ZZL⁺⁰⁹, HKHN08, FHF⁺⁰¹, GD06, HLLS05, mJlZsLyL07, mJlZyL⁺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, Din00, ENM⁺⁰⁴, GT03, HFHL06, JPF⁺⁰⁰, KG02, Kró03, LLA01a, LL01, MT03, PFC03, SMG09, TBG00, SWR06]. **chains** [Cri04, CA07b, DLHC06, MMLC05, MSR04, VM02, XLT07, ZM06]. **chair** [RP09]. **chalcogena** [HKHN08]. **chalcogenides** [JT06]. **challenge** [FKRE08]. **Challenges** [Fie02]. **challenging** [BS06, NGTB03]. **chameleonic** [PA05]. **Change** [KIFK07, OFIK09]. **changes** [HHP04, JO02, Kar06]. **channel** [CXZ⁺⁰⁹, FCP^{+04a}, FCP⁺⁰⁵, HSMT04, MCR08, RAGLL09b]. **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, TSMNG01, YPNE09]. **characterizations** [LS08a]. **characterizing** [Wou00]. **characterizing** [PHJ⁺⁰⁸]. **Charge** [CM09, HT05, JKL08, MZ05, SWM04, ZY01, BB05, BSP06b, Chi03, DWC⁺⁰³, ECM⁺⁰³, FHRR07, GY08, GDV03, GGLR00, GY06, GHBB04, HMOG07, IC08, Jac09, JVK09, KS01a, LFZS04, LLS03, OR05, PB04, PMB04, PP08b, PMPGP05, RLER05, RSN⁺⁰², SL09, San01, SKSH07, SHSF05, SRB02, SvDS01, TCT03, WSM⁺⁰⁹, WM04, XL02, XLT07, YK08, ZBS03, ZH08, SDCG02]. **charge-based** [HMOG07]. **charge-density** [ECM⁺⁰³, XL02]. **charge-scaling** [GY06]. **charge-transfer** [GGLR00, LLS03, ZH08]. **charged** [PPYS08]. **charges** [BSC⁺⁰¹, BCNs07, CR09a, CGBF05, DVP⁺⁰², GHBB04, HS01, JBB00, JJB02, KGL07, KC01b, LMV07, PGG06, SR09, TBSM09, TGGP⁺⁰⁰, UBDPJ04, WMS06, XLT07, YOB⁺⁰⁸, dSGCG00]. **CHARMM** [BBM⁺⁰⁹, HNL08, HMD06, JKII08, LLL03, MM05, MMY07, PB04, PMB04, WHG⁺⁰⁷, WRBV03]. **CHARMM-based** [WRBV03]. **CHARMM-GUI** [JKII08]. **CHBr** [ZWL⁺⁰⁵]. **CHCl** [LDT^{+02a}, ZLLS04b, ZLLS06a]. **CHCLOHF** [YLWL09]. **Chebyshev** [II02]. **chelation** [TFZRG01]. **Chem** [Bof01, HNWF12, Kne05, KWK⁺⁰⁰, Qua01, Van08, WHG⁺⁰⁷]. **Chemical** [BHTCG07, BBC⁺⁰⁵, GCB03, HLS07, Jac09, MGMM07a, PBF07, PYCD03, PYS05, WPS02, AM07, AGMPRG⁺⁰⁸, ATH⁺⁰³, CZFH07, CDD⁺⁰², CWWS07, DF06, DBS07, DA01, DPM09, DSS03, DMN05, Dra00, DHW⁺⁰⁷, Fau01, FVB08, FR06, FLK⁺⁰⁷, FK07b, FHF⁺⁰¹, FO04, GR07, GGB07a, GGB07b, GBB07, GS04, HWFN01, HHP04, JHZ09, KFNH08, Kau07, KBL08, Kle03, KIM⁺⁰⁹, KC01b, KGD06, LWK08, LZZC09, LHP01, LDTS07, LKA01, Mat03, MA05, MC06, NRKH02, OYH05, OKH⁺⁰², PPXP01, PAS08, 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, Woo01, You11, tVBB⁺01, APG05, BWM⁺09, BT00, BMRDB01, BS06, BSJ01, CMaGL⁺04, CFS⁺08, CPUGD09, CMGDAC⁺07, CMCB08, CMA⁺08, DBM03, FJP07, FKRE08, GDPCPU07, GDPP08, GdSuM⁺07, GdAcV⁺07, KSB⁺02, KBA⁺04, KJVW08, KYL03, KC01a, LX07, MGCA07, MR09, MBP09, MMRVH07, MPF00, Nye07, OTL08, SH07, Sha07, SBB02, SGD06, TKH07, Vis02, Ano01c, Ano04b, LB99, Lip00, Sta00]. **chemistry-based** [SBB02]. **chemists** [Pra01]. **Chemometric** [HPL03, MRS09]. **chemometrics** [BLF02]. **chemotaxis** [FC06]. **CheY** [FC06]. **CHF** [UTT⁺04]. **CHFOCHF** [YLWL09]. **Chichester** [Lip00]. **chief** [Lip00]. **CHIMERA** [NSU⁺02, PGH⁺04]. **chip** [Höf05]. **Chiral** [ZPL07, CGMPT⁺08, Sza08, ZOJ⁺06]. **chirality** [CGMPT⁺08, PDC⁺08]. **chiraly** [ST04]. **chlorinated** [DA01, WDZS07]. **chlorine** [mJIZsLyL07, mJIZyL⁺08, WLL07a, XLL⁺02]. **chloro** [JKM08]. **chloroform** [CCK01]. **chloroform/water** [CCK01]. **chlorophylls** [LKT04]. **Choice** [Duk01]. **Cholesky** [SKDO08]. **chorismate** [HHBH00]. **chromium** [RRS06]. **chromophore** [DHM⁺03, HFS⁺07, KHF⁺09, XZ05]. **Chun** [Ano06c]. **CI** [Ano01b, DHM⁺03, HFS⁺07, HKHN08, IK00, dSVA⁺09]. **Cieplak** [Ano06c]. **Circular** [AB08, MM00, HKHN08]. **cis** [DMN05, GRO⁺03]. **cis-diammineplatinum** [DMN05]. **cisplatin** [BZL05, RP04, WM01]. **CL** [FKŠ⁺09, CRC⁺08, DMN05, GZ07, Han01, HYA02, HTN03, HZ09, Hua09a, mJIZyL⁺08, KBL08, LF02, Mar03, RB01, STC⁺08, WLLS04, WDZS07, XFF06, ZY01, ZL09b, BS03, HLLS05, mJIZsLyL07, RFSS06, SLL⁺04a, WLLS05, YLW⁺08, YLWL09, ZWL⁺05]. **class** [CKR08, EBD⁺01, LL07, VIP⁺06, YNW05, hYDN⁺08, Car02, PCS04]. **classes** [CLF⁺09, KH06, QLHL09, XSHC06, XLC08, XWC09]. **Classic** [SRE08]. **Classical** [ATBLS04, COL⁺06, DK01, LLM09, MA05, Nil09, RP07a, STH02, Zho06]. **classification** [GDPCPU07, dGWH01]. **classifier** [CLF⁺09]. **clathrate** [EM03a]. **clay** [ATH⁺03, DJT08]. **cleavage** [CLXC02, NLL⁺09]. **cleavages** [XWXC08]. **cleft** [SPT⁺03]. **closed** [DSB⁺02]. **closed-shell** [DSB⁺02]. **closo** [JRJ01]. **closure** [CSJD04, DLSVY00, Mak08, SWR06]. **Cluster** [AHGK09, Cri04, BR04, BP01, BGJ01a, BWI⁺02, IN08, JBGK08, KKJH08, KSTC01, LMJ02, LWX07, LYS08, Mck07a, MS01, Mor02, NK06, PSF⁺08, SSB07, VDM06, WKYU01, Whe08, WJX⁺08]. **cluster-continuum** [WJX⁺08]. **cluster/adsorbate** [BWI⁺02]. **clustered** [FPN⁺05]. **clustering** [CCWH02, FKZ09, LZ05a, LOL⁺08, RLA01, ZS04]. **clusters** [BP00, BACJCT01, CGG06, CAG07, DSB⁺02, GBBH09, HXD08, HYR06, JHMB⁺09, JHMB⁺11, JG03, KGL07, KDG⁺09, KZW⁺05, LML⁺00,

LWLS07, LJS05, Mck07a, Mck07b, NBJ04, OSHS03, OS08, PBZ00, Pul05, QB05, SCC04, SYC08, SW06, WLL01, WZZ⁺09, WCS09, XZ04, YCS07, ZLJS03, ZXL⁺04, ZWC⁺09, ZXY03, ZGXX06, ZX09, ZB07, Est07]. **CM1** [UBDPJ04]. **CM3** [UBDPJ04]. **CN** [LW04a, TJM⁺03, TYN05]. **CO** [GD06, PLC08, RD00, TJM⁺03, VS02, KT08, ABYM08, DLD⁺02, FLK⁺07, PBZ00, SS05, PLC08]. **co-ligation** [KT08]. **CoA** [LLL⁺08]. **coagulation** [PDP02]. **Coarse** [CA07a, EBAN07, VTT⁺08, CP09, DR07, DJB02, HXLS09, MBC08, PSHP08, SBJ08, WWL⁺09]. **Coarse-grained** [VTT⁺08, CP09, DJB02, HXLS09, 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, LZC09, Whe08]. **coenzyme** [WC08]. **cofactor** [Mck07a, Mck07b]. **cofactors** [Ano06b, CPM03]. **Cohesive** [VP08]. **coil** [OCP02]. **coiled** [OCP02]. **coiled-coil** [OCP02]. **collagen** [PP08a, PRKP05]. **collagen-like** [PRKP05]. **collapse** [Mei02]. **Colle** [IKN08]. **collections** [CDD⁺02]. **Collective** [CCSJ00, HSWN01, LV08, SWR06]. **collide** [CKF01]. **collinear** [Van02b]. **collision** [VW00, VW04, TYN05]. **Collisions** [Pan07]. **collocated** [CJDK09]. **collocation** [CKR08]. **collocation-based** [CKR08]. **colony** [CLZ⁺09, CLZX09]. **comb** [LAEL01]. **comb-like** [LAEL01]. **Combination** [MH08b, DLD⁺02, GHH07, HSWN01, KKS04, dSR08]. **combinations** [ZOJ⁺06]. **combinatorial** [AL01, GD09]. **Combined** [CYM02, GWM08, KBLP09, RG02, ZKZ⁺07, BAL⁺01, BCNs07, BME05, COS01, DPT03, Der09, FSFK05, KH01, KM00, LMCD09, MC06, Oos09, TCR⁺02, VMF⁺03, WX09, XLZ08]. **Combining** [MBC08, SS00, HTKG08, KN04, LLZL09, ZMZ09, KK08b, LEK07]. **comblike** [LZA02, ZALMG03]. **CoMFA** [JFG04]. **Comment** [CPML08b, JW12, Kne05, Qua01, Van08, Bof01, CSD05, WM12, vLBBR12]. **Comments** [MBP09]. **Common** [ZAT07]. **commonly** [ESP04, SCF⁺09]. **Comp** [HNWF12, Kne05]. **compact** [Kri09a]. **comparably** [PB02]. **Comparative** [CCP04, GHLK⁺02, LS02, SBJ08, SCF⁺09, Sto05, VMA03, CMD⁺04, FC06, FO08, GM01, HLMR06, JFG04, KS01b, LPK07, McD08, PHKG07, PMM05, TBG00, WC09, EBL⁺08, JHZ09]. **compared** [IO08, JČHS07]. **Comparing** [JCL05]. **Comparison** [AEE⁺03, Bou00, CV09, DB07, DLG00, GGLR00, Kr603, SL06, SDL07, TCR⁺02, WMGK07, WMW03, YLL⁺09, ZCL09, AE06, BL05, FOL⁺04, FDSA00, GDPCPU07, Gra07, HRBKB03, JARM02, LC07, LOL⁺08, LZF⁺09, MZ05, MS00, MST⁺08, MC06, PK04, PS03, RDM⁺08, SBLK01, ŠBL05, SSB07, WB04a, WB04b, WB05, BRDC02, CCT⁺03, COL⁺06, LKT04, NCO⁺05, ONHN00, PSF⁺08, SPDS01, SL04, SKK⁺07, WMW04, YKK09, ZGFL01, ZOJ⁺06]. **Comparisons** [GPK05]. **COMPASS** [MSR04]. **compatible** [BSDM04, KH06]. **competing** [HA04]. **competitive** [FG03].

complementarity [EKB02b]. **Complete** [BT00, MLL^{+08b}, Pog03, PRT⁺⁰⁷, PRT⁺⁰⁸, MC06, Var09, WMRW⁺⁰¹].
completeness [AHK02, MV06]. **completeness-optimized** [MV06].
Complex [DFGB09, AS06, Bac09, BRS00, BRS01, GC04, HDF⁺⁰⁷, HDO⁺⁰², HMK02, IV04, IvSV06, Ish04, JLHF03, Kle02, KVS⁺⁰⁶, LB05, LDL⁺⁰⁹, MM03, MCF05, MY08b, MY08a, NHN06, Pac06, ZWB09].
complexation [AGI⁺⁰⁷, HT05, LMMW04, SRK⁺⁰⁰, SLRC01]. **complexed** [Pin03, SDM02, WCF04]. **Complexes** [APG05, AB00, Ano06a, ACM⁺⁰⁶, BTP09, BR04, BL06, BM00, BGC⁺⁰⁹, BZL05, CZ05, CG03, CBC⁺⁰⁸, CSB08, CBH⁺⁰³, DPT03, DF04, FRS05, FO08, FRLN09, FKŠ⁺⁰⁹, GTC06, GL04b, GM01, GPSP06, GPK05, Gri04, GZM09, GWL07, HLLN06, HRG07, IN08, IO08, IGL07, JMD⁺⁰², JD09, JČHS07, KT08, KRM⁺⁰², KJP⁺⁰⁷, LL00, LHJ⁺⁰⁶, LPP06, LH02, LMGR06, LLS03, LMMW04, LWZ09, LZP⁺⁰⁹, LS05b, Mas04, McD08, MHJS06, MSBS01, MLL^{+08b}, NyHN06, NR04, NMAT01, PGG06, QTdG⁺⁰⁸, RPNJ07, RMP01, RRFC⁺⁰³, SG07a, SCF⁺⁰⁹, SBH02, ST06, SVV⁺⁰⁸, TGGP⁺⁰⁰, UM03, VS02, VMA03, VL00, WB07, WWT08, Won09, ZY01, ZBS03, ZWY⁺⁰⁹, ZTS09, dVB01]. **complexes*** [GK09]. **complexity** [BT00, PK05, XSHC06]. **Component** [KBA⁺⁰⁴, CCT⁺⁰³, GPSP06, JMD⁺⁰², PVdJB00, PV03, SH02, SM08b, Van02b, WGo2]. **Component-based** [KBA⁺⁰⁴]. **Components** [KJVVW08, Car02, LL07, TGGP⁺⁰⁰]. **composition** [HM06, KWHH07, LL07, PAS08, XSHC06, XLC08]. **Compound** [CN05, BR07, HBM06, RD00, XZ05]. **compounds** [ACLD03, BB08, BLO⁺⁰², CYM02, DA01, EBDPM00, EDAJ04, EBD⁺⁰¹, FJ08, FROD08, FO04, Gol09, Gor01, JLHF03, KFD06, LLA01a, LLA01b, LLA01c, LLA01d, LLA03, LD05a, LWK08, LTF⁺⁰⁷, LWH06, LCDA03, LCGA03, LCA03, LJZ⁺⁰⁷, LLM09, MDI04, NBTN04a, NBTN04b, PZWG⁺⁰⁴, PYCD03, POJ01, RUPH06, SJJ⁺⁰⁴, ST01, TTBM09, YCW⁺⁰⁹, YSA⁺⁰³].
Comprehensive [LF02, ZL09b, ZB07, DLR⁺⁰⁸, JPF⁺⁰⁰, ŠBL05].
compression [BG07, MBWP03]. **comprising** [Rud05b, Rud05c]. **Comput** [Bof01, Qua01, Van08]. **Computation** [BLL⁺⁰⁶, Car02, CDD⁺⁰², FZL07, GS09, LFEeL06, TNS00, ATMK03, Gon07, NKIS02, PAS08, RK05, WZXY07, ZCZ03, vW06]. **Computational** [Ano01c, Ano04b, Ano05b, Ano06a, Ano06b, Ano06c, BLMS08, CZ05, CPUGD09, CMGDAC⁺⁰⁷, CMCB08, CG05, CA07b, GBL⁺⁰⁵, GDPCPU07, GdSuM⁺⁰⁷, HMK02, LKJ⁺⁰⁴, LB99, Lip00, MW00, MFR07, OY03, Pac06, SPGS08, vRS98, Sta00, TMBM02, WB04a, WWC⁺⁰⁵, WXK08, You11, ZOJ⁺⁰⁶, ZWB09, Bac04, BG00, BAL⁺⁰¹, BTP09, BMRDB01, BZL05, CMLS05, CFS⁺⁰⁸, CBC⁺⁰⁸, CJS⁺⁰³, CRH⁺⁰⁷, FG03, FJP07, FD03, FKRE08, Gan09, GD09, GDPP08, GdAcV⁺⁰⁷, GGB07a, KYL03, MCF07, McD03, MH08a, OTL08, OY01, OSA06, Pan07, PMM05, PWFS01, PRS04, RGG08, SF07, SM03, STCJ08, TD08, Vis02, VZM⁺⁰⁸, WSM⁺⁰⁹, WOC⁺⁰³, YT03, YT04, YDWS06, ZZ08, ZGZX07, ZTP⁺⁰⁸, ZM06, Woo01].
Computationally [KM00, KFZ03]. **Computations**

[Bou01, Dib05, CLP⁺05, GPK05, Lu09, ME06, Pog06, SMZW05, TT08].
compute [BDW00, RKA⁺09]. **computed** [PFJ⁺03, PK05, TDH06].
computer [HFSD03, Höf05, NK01, PPXP01, PHJ⁺08, TRS02, UIHN09, VB07, VKCK09, YNZ⁺08, Zer08]. **Computing** [HHW⁺03, WL00, BHH⁺09, DGHR02, DP04, DK01, GLD08, HHS⁺05, KFB05, LM03, MA09, ZP03].
CONAN [SSHT03]. **concave** [Won09]. **concentration** [GGT08]. **concept** [LSY02, Rao00b, Rud05a]. **Conceptual** [VB09]. **Concerning** [FG03, Bor03].
concerted [LFS⁺07, Mck07b, NSB08, LLKC06]. **condensed** [CLP09, DGI⁺08, DWC⁺03, FM00, GLMV09, Mor02, SDvG01, ZSK07].
condensed-phase [DWC⁺03]. **condition** [SK08]. **conditions** [BVW04, CEP07, HH04, WM06]. **Condon** [Ama02a, LMCD09, TP01b].
conduction [SM06]. **conductor** [DHW⁺00, FZL⁺06]. **conductor-like** [DHW⁺00, FZL⁺06]. **Configuration** [LSAS01, SLRC01, ASS⁺02, BMRF01, DLD⁺02, KBT03, LWX07, MLL06, PRSMM02, PRSMV08, SSL02, SWZS04].
configurational [HDF⁺07, HTKG08]. **configurations** [MM03, MABM09].
Conformation [GS04, BY06, BR03, BLB09, DPM09, LXL07, PFJ⁺03, YL06, YZ06].
Conformation-dependent [GS04]. **Conformational** [AJNG01, AZS⁺04, BLF02, DSS03, HW09, KK09, LRI⁺02, LGB⁺09, OYK⁺09, OM04, PSDM00, SH09, SMGE08, SSHT03, SR09, TTB01a, TTB01b, WHRG08, WW04, BISB02, BMTSC01, BAH⁺02, CN03, CSJ01, CvG08, CS01, CCP04, CSRST04, CKT⁺08, DDKV07, DSR⁺07, ECA06, FGR07, FC06, FD03, GT03, GSB09, HYA02, IB04, IZA06, JW06, JO02, KB02, KK08a, KH01, Kle02, KK01a, KF08, LFKL00, LKJ⁺04, LCKL05, LJKL08, MFB04, Mak08, MH08b, MA05, MGJAARC00, NKIS02, OML⁺00, OGH05, PRT⁺07, PRT⁺08, SPL⁺02, SWBM08, SHBD05, SD09, SSBE06, WCK00, YXL⁺09, ZA07, CG03, HJCP01, JPF⁺00]. **Conformations** [NHH05, CLWL09, CIB05, yCkHmY08, DBM03, ENM⁺04, FWH⁺07, GBB07, GB04, HDO⁺02, HP05, LZKT04, MW00, OFB08, OKH⁺02, PC00, PFC03, Rao00b, RP09, TLKT00]. **conformers** [HS00, HHP04, KAS⁺07, PG01, RSSKB03, TT02, WD04, YXL⁺09]. **Congo** [SRK⁺00]. **conical** [IK00]. **conjecture** [Pog03]. **conjugated** [BG00, CZ05, DDBP09, LYS08, LC09, LFR07, WJ00]. **connectivity** [EDAJ04, Pog06]. **conquer** [AKN07, MLJ03, vdVGDM00]. **consensus** [GP06, JMD⁺02, LLL⁺08, RHL09]. **Consequences** [RSS09]. **considerations** [GRCD01, PB05]. **Consistent** [RP02, BWI⁺02, ECM⁺03, KK08a, KBN02, NUH02, SMD02, VTT⁺08, WM04, XL02]. **Constant** [MCM04, DRMD03, Sch00, Vas02, WLLS05, WLL⁺07b]. **constants** [Chu07, FCW06, GGB07a, GGB07b, HWFN01, JHZ09, Kle03, MMLC05, MGLL03, MDI04, PJPJdPRMI07, RRFC⁺03, SLL⁺04b, SFRS01, TLOG00, WDX⁺02, WZXY07, ZXY08]. **constrained** [COS01, EC06, LFKL00, MM00].
Constraining [AM09, HSWW00]. **constraint** [BL09, FS98, FS00a, KvGH01, YXC⁺07]. **constraints** [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, LWV⁺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, HHS01, SM08b, PDC⁺08]. **Continuum** [FCP⁺04b, MGLO03, ABWT09, BCIB05, CFK08, COL01, CCT⁺03, COL⁺06, FKL⁺06, FEVM01, FBLO08, GS02, GWS⁺02, HC08, HS01, HHP04, KKS04, LRI⁺02, LJ04, MWL⁺08, Pom04, RSP03, Sch00, STSF02, TJE03, VP09, WJX⁺08, YÇBM00, 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, MGLO03, RM07, SWV⁺05]. **Control** [Kar06, DB06, LR06, MN02, RS05]. **conventional** [WMW03, WMW04]. **Convergence** [KGN07, LST08, GG09, LTV08, LJ04, Mas04, Rud05a, Rud05b, Rud05c]. **convergent** [PAS08, Zho06]. **Converging** [GC04, KF02b]. **conversion** [CC09, 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, KSU03, LPK07, NKIS02, 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, GAI06, Gri06, HK08c, HK08d, IKN08, LBT07, MGLDS00, Mue01, QCK01, QCK02, SPDS01, STSF02, TKH03, WX09]. **corrections** [BF07, Gri04, KSS08, WB07]. **correctly** [LF04]. **corrector** [Kol04]. **correlate** [Kle03]. **Correlated** [GBB07, BWV⁺08, BLT03, DBM03, GPSP06, KMA⁺07, PFB05, TBG00, WMW03, WMW04]. **correlating** [NSO⁺07, SNM⁺06]. **Correlation** [LRWG03, TDH06, AAP00, AGI⁺07, AS00, BL00, CKT⁺08, EL09, FDM00, GKTS04, HN02, HR08, Hir08, IKN08, JJK⁺00, JSHG07, KGN07, KK08a, KC01b, LMJ02, Mat03, PJPJdPRMI07, PMC⁺08, SRE08, TKH07, WMW03, WL04, YH09, dSGCG00, WMW04]. **correlations** [DR09, HHW⁺03]. **Correspondence** [RLRE01]. **corrphycene**

[NyHN06]. **COSMO** [EK06, ELK⁺09, KEH⁺02]. **COSMO-RS** [EK06, ELK⁺09, KEH⁺02]. **COSMOS90** [SO07]. **costs** [SSL02]. **Coulomb** [WMW04, BWP07, Nee03, WMW03]. **counterions** [JD09]. **counterpoise** [GAI06]. **counting** [HYT05, LM03]. **Coupled** [BSP06b, MO01, CXZ⁺09, DOSG06, IN08, KSTC01, LMJ02, LYS08, PSF⁺08, SSB07, WKYU01, Whe08, XWC09, SMAv00]. **coupled-cluster** [IN08, KSTC01, Whe08]. **coupling** [CR08, DXW08, GdAcV⁺07, KTM02, KBLP09, LB08, MDI04, PJPJdPRMI07, QTdG⁺08, RI08, RLDI09, 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** [ALT06, GLD08, PSDM00]. **Critical** [GT03, BMLV04, BLN01, BAÅ07, CRC⁺08, CKMC04, FMPS08, LFR⁺04, MP03b]. **cross** [Gan09, MY08b, MY08a]. **crosscorrelation** [HWDB03]. **crossed** [BAL⁺01]. **crossing** [LI07]. **crossings** [LSG06]. **crossover** [KRLD09]. **crown** [GLRL02, HDO⁺02, LWW⁺06, ZWY⁺09]. **crown-shaped** [LWW⁺06]. **cryptand** [HN02]. **cryptand** [WWT08]. **Crystal** [KOFF09, Van02a, DPT03, EL09, HN02, KP05, TD08, VVBV02, vDSSvA04, vEMK01, vE01, DRMD03, FROD08, PZWG⁺04]. **crystalline** [AS00, CADW03, JB04, PZWG⁺04, Wil01a, ZLD09]. **crystallographic** [RON02]. **crystals** [BCF⁺09, CC07, FÁ01a, GAdGM08, GBJ03, PMC⁺08, RD06, WMS06, Wil01b]. **Cs** [GWL07, GLRL02]. **CSA** [NCO⁺05]. **CSOV** [GPSP06, PMPGP05]. **Cu** [BTP09, GPSP06, Sha02, HSF08, NK06, TDK07, WCS09, ZTP⁺08]. **CuN** [ZX08]. **cuprates** [MDI04]. **Current** [NYTH09, CDPL09, Vis02]. **curvature** [TRS02]. **curved** [ABWT09]. **curves** [BBI⁺09, MM07, SSS⁺09, ZLY07]. **Customized** [BDW00]. **cut** [BME05]. **cutoff** [GGT08, KLM⁺09]. **CuX** [KBL08]. **cyanines** [BG00]. **cyano** [PA05]. **cianoacetylene** [YDWS06]. **cyanobiphenyl** [CC07]. **cyanoboranes** [WCW08]. **cyanomethylidyne** [WDS06]. **cycle** [ZAT07]. **Cyclic** [KJP⁺07, BGJ01a, CLA⁺00, FKM⁺06, FKM⁺07, JBGK08, LXL07, OYK⁺09, VVS07, WOC⁺03]. **cyclic-AMP** [FKM⁺06, FKM⁺07]. **cyclization** [PWFS01]. **cyclizations** [SGS03]. **cyclo** [TDK07]. **cyclo-Cu** [TDK07]. **cycloalkanes** [SSBE06]. **cyclobutane** [QZZZ03]. **cyclobutene** [SRE08]. **cyclohexane** [MT03, RP09]. **Cycloketones** [LLA01b]. **cyclononane** [SSBE06]. **cyclononatriene** [ZSE08]. **cyclooctatetraene** [CPFL02]. **cyclopentadienyl** [ML00]. **cyclopentene** [SURG06]. **cyclopeptidic** [FL07]. **cycloreversion** [QZZZ03]. **CYP2A6** [VB09]. **cysteine** [CN05, MOP⁺07, PMM06]. **cysteine-6** [PMM06]. **cysteines** [CFR06]. **cytochrome** [AST06, ATBLS04, HBM06, JKL08, LCC09, OYH05, OON01, ZAT07, BS06]. **cytosine** [KKMMS04, MDA08, MHS05, MH08a, SBI08, SG07a, SC01].

cytosine- [MHS05]. cytosine-5-acetic [MH08a]. CZ [CRC+08].

D [IS03, PF06, SHBD05, AGO+02, BAH+02, CPC+00, DDBP09, DMC05, FROD08, GDPCPU07, GdSuM+07, GdAcV+07, HP05, LW04b, LXZ06, LW06, MP03b, OYK+09, RSSKB03, RGP+07, SFC04, YNW05, hYDN+08, ZTS09, vDSSvA04, TGLL07]. **D-** [AGO+02]. **D-arabinonate** [RGP+07]. **D-arabinonohydroxamate** [RGP+07]. **D-Epitope-Explorer** [SHBD05]. **D-erythronic** [vDSSvA04]. **D-galactose** [RSSKB03]. **D-QSAR** [DMC05]. **D-RNA-coupling** [GdAcV+07]. **D/** [PF06]. **D180** [NYK+09]. **d2_cluster** [CCWH02]. **damage** [FPN+05]. **dangers** [MBP09]. **data** [ASWG07, BRDC02, BK00, CDD+02, CRGN07, FOK+04, FM00, HHJ03, HSWN01, KMH02, KMA+07, LEK07, MBWP03, MMP+07, PFJ+03, PF06, RLA01, RRS09, RRS09, RON02, SY09, SFC04, WG02]. **database** [DPM09, LFKL00]. **databases** [BR07, PPXP01]. **dativ** [FH01]. **David** [Woo01, Ano05b]. **day** [GR07]. **DD** [ZLY07]. **DD-curves** [ZLY07]. **Dead** [YFS07, Adc04, GLD08, KUB07, PSDM00]. **Dead-end** [YFS07, Adc04, GLD08, KUB07, PSDM00]. **deaminase** [MDA08]. **dearomatization** [HT05]. **debates** [Nye07]. **decarboxylase** [HLC09, LLL+08]. **decarboxylation** [UTH+03]. **decker** [RPNJ07]. **decomposable** [VZM+08]. **decomposition** [BM07, CBH+03, FK07a, FPG+06, Hir08, KZY09, KN04, LBG08, ML00, SKDO08, TBSM09, TCR+02, ZZL04]. **decompositions** [GPSP06, PBF07]. **decoys** [LZ05a, SRCD03]. **defect** [ZMH+09]. **defects** [JT08]. **Definition** [EA06, LFSB03a, LFSB03b]. **Definitions** [PBF07]. **Definitive** [dOMSL01]. **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** [JJH01]. **dehydrohalogenation** [TT02]. **deletion** [SHH07]. **delineate** [MP03a]. **delocalization** [BY06, BI06, FVB08, FS02, Kar06, MGMM07a, MGMM07b, WMW03, WW03, WMW04, Wan09]. **deltorphin** [OM04, YAÇ+02]. **deMon2k** [GJK+06]. **denatured** [GB04]. **dendrimeric** [SCG04]. **densities** [GY08, GBJ03, HSWW00, KCK+08, LMV07, RLR+04, VZVG06, Van02b]. **Density** [BP01, FG02, Han01, JČHS07, KWK+01, KWK+02, MSBS01, QZZZ03, QZL+04, VL00, WCW08, AB00, ABYM08, AEE+03, ASY01, Bac09, BP03, BMLV04, BB08, BAAÅ07, CLP+05, CRC+08, CFK08, CRS05, CR08, CSB08, CAG07, CPML08a, Cul04, CGSdST06, DVP+02, DVRP+03, DF04, ECM+03, FCW06, FZL07, FDM00, FS04, GHLK+02, GLRL02, Gri04, Gri06, GBBH09, GHBB04, HGMB04, HLS07, HNWF07, HNWF12, HN02, Hir08, Hol05, II02, ION07, IN08, IB04, ITN+05, IS07, JNV08, Jac09, JCA+02, JFG04, KGL07, KRM+02, KN04, KSS08, Kle03, Kni00, KZW+05, Kri09a, KS01b, LRI+02, Leh06, LV08, LMB08, LMGR05, LLS03, LWH06, LKT04, LF02, LLZL09, LDL+09, LZP+09, MP03a, MW09, MS00, NK06, NTH09, NAT07, OKE+02, PSF+08, RB01, RK04, RLER04b, RDM+08, RR05,

RZWS07, SH07, SZT08, SPT⁺⁰³, SCF⁺⁰⁹]. **density**
 [SLRC01, SSB07, SW06, TBG00, TST⁺⁰⁸, TKN⁺⁰⁸, TKH03, Van02b,
 VMA03, VBS09, VC04, VKCK09, WRP⁺⁰⁶, WB07, WZY04, WMRW⁺⁰¹,
 WL02, WCHW09, WM04, WCL05, WZXY07, WM01, XB08, XL02, XPW09,
 YTH01, YL09, YK08, YYW07, YLL⁺⁰⁹, ZZL04, ZH08, Zho06, ZM03,
 vGGB00, Haf08, LWK08, MW00, XYN⁺⁰⁶, GM01]. **density-functional**
 [HNWF07, HNWF12, LLS03, LWH06, TST⁺⁰⁸, XB08, Haf08].
density/polarization [YL09]. **deoxyguanosine** [MM02].
deoxyribonucleoside [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, LDL⁺⁰⁹, LSW⁺⁰¹, MML02, MW09, MY08a, NTH09,
 ONHN00, PSF⁺⁰⁸, TST⁺⁰⁸, TKN⁺⁰⁸, Whe08, WC08, YH07, ZH08, ZM03,
 vGGB00, PMM05]. **depiction** [ZTS09]. **deposit** [JG03]. **deposition**
 [UNM⁺⁰¹]. **deprotonated** [Mas04]. **Derivation**
 [EBD⁺⁰¹, JFG04, TT05, TTB01a, EBD⁺⁰¹, HZ06a, Tor02, Tot04].
derivative [CNN07]. **derivatives** [BT00, Bor03, BC06, CJK⁺⁰², COMR⁺⁰⁴,
 DMC05, DOSG06, FL08, GLRL02, IS03, PSF⁺⁰⁸, PA05, QCK01, QCK02,
 RP09, SPGS08, SGPS09, Sch00, STC⁺⁰⁸, TNS00]. **derived**
 [GBJ03, HSWN01, Ish02, KŠB09, KS06, KFNH08, MLJ03, SvDS01, TBSM09,
 WMS06]. **Deriving** [RPMP03]. **desaturation** [BBSS06]. **descreening**
 [MTE04]. **describe** [DDBP09, IDMC09, MSH^{+06b}, RLDI09, SBI08].
describing [CMaGL⁺⁰⁴, HK08a, HK08b]. **Description**
 [ION07, MHT01, BUMCMRL00, BME05, CLWL09, CHRL09, Gri04,
 HGMB04, SM08a, VMA03]. **descriptions** [SB08]. **descriptor**
 [CDS09, RSS09, TCSM03, XYN⁺⁰⁶, ZNLL07]. **descriptors**
 [AGMPRG⁺⁰⁸, BAÅ07, DA01, EDAJ04, HM08, HMMS09, Jac09, LXW⁺⁰⁹,
 MGMM07b, RUPH06, Tie09, TTBM09, Wou00]. **Design**
 [AG03, KV00, BSP06a, BMTSC01, BLMS08, CRH⁺⁰⁷, CMBC08, DB06,
 DHW⁺⁰⁷, DHW⁺⁰⁹, GHMP03, Ham07, HM06, HLTL09, HLM05, JGVF05,
 LFBSK07, LZ05b, LFS⁺⁰⁷, MWE02, NHH05, PS09a, SPGS08, SRS07,
 SHM04, STCJ08, VGGMM05, VZM⁺⁰⁸, YFS07, ZZ08, ZL09a]. **designed**
 [GT03]. **designing** [GDV03]. **Desirability** [CMBC08]. **Desirability-based**
 [CMBC08]. **desolvation** [HMOG07, SWV⁺⁰⁵]. **Detailed** [PB05, WRBV03].
details [GGB07a]. **detecting** [BHH⁺⁰⁹]. **Detection**
 [WHH⁺⁰⁶, BAL⁺⁰¹, CMCB08, OYH09]. **determinant** [GS09].
determinants [BCP03, Bou00]. **Determination** [BLT03, CFR06, CR08,
 DLD⁺⁰², FSS00, Vas02, BL08, BR03, BCNs07, BdPRMAI00, CC09, Chi03,
 CAGR08, FAR02, GCCVB00, HP05, Mar03, MGLDS00, MM07, PC00,
 PFC03, PABK03, RI07, RTG00, SCF⁺⁰⁹, TBSM09, vDSSvA04].
determinations [YXL⁺⁰⁹]. **determine**
 [DDVD09, KUB07, OO08, RI08, YH06]. **determined** [OYH05, TDH06].

determining [BY06, DV02, LR06, PHJ⁺08]. **Deterministic** [LS05a].
detonation [JWB05]. **detoxification** [ZWS⁺09]. **developed**
 [CRS05, KMH02, RG08]. **Development**
 [ATMK03, BGJ01a, HHJ03, IS07, KSB⁺02, KOML08, KVL⁺04, LAT05,
 LK03, MSR04, MRC03, WWC⁺04, WWC⁺05, WS05b, XYN⁺06, Yan04,
 BA08, COS01, CMGDAC⁺07, KLB03, NG04, BG03, IKYM09, SM08b].
developments [FCP⁺04b, HS07a, SMD02]. **DFT**
 [BRLS12, ASDP⁺06, ACM⁺06, BWP07, BPC01, BP07, BSB05, BM08, BB08,
 BE07, BRLS08, BBSS06, BZL05, CMJ08, CCCJ09, CHA⁺07, CG06, CS03,
 CMA⁺08, DGD⁺05, Der09, DDBP09, ESP04, EKO⁺01, EBL⁺08, FO08,
 FO04, FKŠ⁺09, GCCVB00, GKH05, GPSP06, GKTS04, HLLN06, HT05,
 HSWW00, HK07, HZ09, Hua09a, JPF⁺00, Kle02, Kle03, KTM02, Kri09a,
 KPZK06, LMV07, LYK⁺04, LDC⁺07, LWLS07, LS08b, LWZ09, LS05b,
 MML⁺06, MOP⁺07, MGG06, MBWP03, PFJ⁺03, PMPGP05, PMM06,
 RM00, SBI08, SWBM08, ŠBL05, SN06, SCG04, SSBE06, SRB06, Tie09,
 VS02, VB09, WMGK07, WLX⁺05, WWT08, WL09b, XLL⁺02, XKG⁺05,
 YS00, YK08, ZSE08, ZKZ⁺07, ZWS⁺02, ZWY⁺09]. **DFT-D** [DDBP09].
DFT/MRCI [KTM02]. **DFTB** [ECM⁺03]. **di-** [CU01, GBB07]. **di-arsenic**
 [KS05a]. **diabetes** [PS09a]. **Diagonalization** [LSAS01, BdPRMAI00, PU09].
diagram [Hir08]. **diamide** [HHP04]. **diaminoguanidine** [BI06].
diaminosilylenes [TKS⁺01]. **diammineplatinum** [DMN05]. **diamond**
 [EKO⁺01, JBGK08, ZMH⁺09]. **dianionic** [OSA06]. **diatomic**
 [ALKH04, FCW06, TLOG00, WWS07]. **diatomics** [Cul08]. **Diatropicity**
 [CdML06]. **diazonium** [EL06, EL07]. **diborane** [wQZsLyZ02].
dibromomethane [LXSF08]. **dicarboxylic** [NHH05]. **dication** [Bac09].
dichlorides [LHP01]. **dichloromethane** [RRZA08]. **dichroic** [MM00].
dichroism [AB08, HKHN08]. **didehydropyridine** [KC01a].
didehydropyridinium [KC01a]. **Dielectric** [HS01, DRMD03, GS03,
 HMWC03, HLLN06, LZZC09, MML02, Vas02, ZFW08]. **Diels** [Hir08].
DIESEL [ME06]. **differ** [SRK⁺00]. **difference** [ALC08, Bie04a, Bie04b,
 BF04, PMPGP05, PZS04, Rud05a, Rud05b, Rud05c, VZM⁺08]. **differences**
 [CV09, GG09, OV03, YZ04]. **different** [ABÅ04, BL05, CEP07,
 CMGDAC⁺07, DSB⁺02, MCF07, MN02, VC04, WM01]. **differential** [DD08].
differently [HSF08]. **diffraction** [HHJ03, dGWH01]. **Diffuse** [GS07].
Diffusion [VW04, BZP09, Bie04a, CCCJ09, Rud05a, VW00, PK04].
difluoroethane [CUS00]. **dihaloethanes** [WFR08]. **dihedral**
 [FKZ09, HK08c, OFIK09, YL06]. **dihydro** [WJX⁺08]. **dihydrodiol**
 [PCMG09]. **dihydrofolate** [GGLR00]. **dihydrogen** [Mck07b].
Dihydrophospholophosphole [CDL06]. **dihydropyridine** [HSMT04].
dihydroxypyridine [YXZ⁺04]. **diiminobenzosemiquinonate** [Bac09].
diiron [BB08]. **diketimate** [GTC06]. **diketonate** [RMP01]. **dilute**
 [HRR05, Kri09b, XZ04]. **dilution** [DA01]. **dimension** [TSMNG01].
dimensional [BP01, Bie04a, CVR08, DHW⁺08, LAR⁺03, LR06, MP03a,
 MVLG06, RSS09, SHBD05, Wan09]. **dimensionality** [CDGS09].

dimensions [AHK02]. **dimer** [CWY09, GYCZ04, Kr603, LZJ03, MMPK01, McD03, NK01, RRCA08, SBI08, SG07b, YTH01, ZGXX06]. **dimerization** [HK07, JJK⁺00, WXK08]. **dimers** [BBI⁺09, FKRE08, GYMN07, LMGO⁺09, NL08, OKE⁺02, Owe05, RB01, VC04, WXK08, ZOJ⁺06]. **dimethoxyethane** [LCGA03]. **dimethyl** [GGGLL05, GWM⁺00, WLL⁺03, WJX⁺08]. **dimethyl-2-iodobenzoylphosphonate** [GWM⁺00]. **dimethylacetylene** [MTB09]. **dimethylallene** [ZPL07]. **dimethylamino** [ZH08]. **dimethylcarbamate** [KKH⁺07]. **dimethylhydrazone** [Lu09]. **dinitrogen** [Ano06a, ST06]. **dinuclear** [SMM⁺08, SDM02]. **diodes** [LFR07]. **diol** [Kle02, Kle03]. **diol-water** [Kle02]. **diols** [Kle02, Kle03]. **dioncophylline** [BMRF01]. **dioxide** [KT08, KZW⁺05, KK01b, gThDjL⁺01, ZLLS04a]. **dioxide-based** [KZW⁺05]. **dioxygen** [BLO⁺02, SSW⁺07]. **dipalmitoyl** [CEP07]. **dipeptide** [BISB02, ECA06, HLMR06, JW06, KK09, LRI⁺02, LL07, PFJ⁺03, Qua07, WD04, YXL⁺09]. **dipeptides** [LSW⁺01, TTB01b, YXL⁺09]. **diphosphates** [PFR04b]. **dipolar** [RI08, San01]. **dipole** [DVP⁺02, EDW07, HN02, HK08a, HK08d, HK08b, KFZ03, MLA00]. **dipole-quadrupole** [HK08a, HK08b]. **dipoles** [DVRP⁺03]. **Dirac** [HDBD04, PVdJB00, TW03, Vis02]. **Direct** [CBS⁺03, CAG07, JJH01, LW04a, TY03, WLLS04, WDX⁺02, YLZ08, GLMV09, HP05, mJZsLyL07, PC00, PFC03, SLL⁺04a, SHH07, SVT09, UKN04, WLL07a, WyLG⁺09, WLL⁺03, XLL⁺02, ZWL⁺05]. **direct-particle-deletion** [SHH07]. **directly** [SFRS01]. **disaccharide** [FKJ⁺01]. **disaccharides** [SRB02]. **DISCO** [ZBS03]. **DISCOtech** [JFG04]. **discover** [LHJ⁺06]. **discovery** [HS07b, KV00]. **discrete** [DXW08, MGLO03, QLHL09, YL06, ZBS03]. **discretization** [Bie04a, Bie04b, RP07b]. **discriminant** [ZHH09]. **discriminants** [FTLV01]. **discriminating** [yCkHmY08]. **Discrimination** [LDTS07, ZPL07]. **discriminative** [WHH⁺06]. **discussion** [CDGS09]. **disilenes** [TKS⁺01]. **dismutase** [PMM06]. **dismutases** [RJLR06]. **Dispersion** [COL⁺06, RDM⁺08, CLZX09, GYMN07, Gri06, JČHS07, KSS08, Lab08, Whe08]. **dispersive** [BCF⁺09]. **dissimilarity** [hYDN⁺08]. **dissipative** [YCX03]. **dissociation** [CJW⁺09, KWK⁺01, KWK⁺02, LS05b, TJM⁺03, WZZ⁺09]. **dissociative** [ABYM08, KKJH08]. **dissolution** [SBG09b]. **distal** [IGNH03]. **Distance** [MML02, RSS09, Ano05b, BL00, Cri04, IZA06, KvGH01, KH06, LI07, LHI09, PYEA03, Sha05]. **distance-dependence** [BL00]. **distance-limited** [Ano05b, Sha05]. **distances** [Var09]. **Distorted** [KS01b]. **distortion** [LMO09]. **distributed** [ASWG07, DGHR02, FOK⁺04, IS07, KMA⁺07, SKK⁺07, TYO⁺02, ZP03]. **distribution** [ACM⁺06, BBP09, CFS03, CV09, CMGDAC⁺07, JVVK09, KS01a, KS02a, LBT07, MZ05, MLG04, PP08b, SK09]. **distributions** [AEE⁺03, BSP06b, Chi03, HLS07, LV08, MFB04, RLER05]. **disulfide** [DWS⁺09, KF03, wQZsLyZ02]. **dithiacyclohexane** [FD03]. **dithiane** [FD03]. **divalent** [GS04]. **diverse** [AGMPRG⁺08, AVS09]. **diversity**

[ZHH09]. **divide** [AKN07, vdVGDM00, MLJ03]. **divide-and-conquer** [AKN07, MLJ03]. **dizincocene** [G XK09]. **DL_POLY** [KSY+00]. **DMPC** [HNL08]. **DMS** [RAGLL09a, RAGLL09b]. **DMS-OH** [RAGLL09a]. **DMSO** [RAGLL09a, RAGLL09b]. **DNA** [AB08, AZM03, BCP03, DLW06, DLWV07, EL06, EL07, FPN+05, FKM+06, FKM+07, JMD+02, JCL05, LW04b, LD05b, LXZ06, MB00, Maz01, PG04, Pin01, Pin03, PSHP08, PSS+04, PSMB05, RTG00, SG07a, SHD+08, WRP+06, WWL+09, hYDN+08, YS00, ZLY07]. **DNA-base** [PG04]. **do** [SRK+00, YJF06]. **Dock** [BS08, CWV+05]. **docked** [NMAT01, ZWB09]. **Docking** [BTLPO3, RGZM09, WS02b, AGI+00, AGI+07, AB09, BS05, BS08, CKMC04, CBC+08, CLH+07, CGBF05, CWV+05, CR09b, GZM09, HR08, HLM05, HW09, KG02, KCL06, LR03a, LCKL05, MKT04, MM03, MCR08, MHL+09, RK05, Ruv07, SBG+09a, TH02, TFN04, TJE03, TP01a, Tot04, VVS07, WRBV03, YK00, Yan04, YKK09]. **dodecamer** [JCL05]. **Does** [RY09, RS07a, RS07b, WCK00]. **DOIT** [SFRS01]. **domain** [IGNH03, JS07a, OO08, PAT+09, PYCD03, PYS05, PC07, PLC08]. **domain-averaged** [PYCD03, PYS05]. **domains** [GCDL+05, PC05, 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, DLRZ09, LMGO+09, Won09, YS00]. **double-stranded** [AZM03]. **doubles** [IN08, WKYU01, dSVA+09]. **doubly** [CHRL09, LDL+09]. **doubly-linked** [CHRL09]. **Douglas** [YH09]. **Douglas-Kroll-Hess** [YH09]. **downward** [LMO09]. **DP** [CDGS09]. **DQ2/DQ7** [KVS+06]. **DQ7** [KVS+06]. **DQ8** [KVS+06]. **drag** [YSJ09]. **Dramatic** [AM06a, KT08]. **dressed** [MW09]. **driven** [MH09, PV03, SVT09, WPS02]. **drives** [LFS+07]. **driving** [AM07]. **Drude** [LLM09]. **drug** [CMCB08, DHW+09, HS07b, LLW+09, MCR08, PPXP01, PFR04a, SPGS08]. **drug-induced** [CMCB08]. **drugs** [BLB09, KEH+02, KC01a, SMM+08, VGGMM05, WM01]. **DsbA** [CFR06]. **Dual** [WyLG+09, WLL+03, ZWL+05, mJlZsLyL07, TST+08, ZZL04]. **Dual-level** [WyLG+09, WLL+03, ZWL+05, TST+08, ZZL04]. **Duan** [Ano06c]. **due** [Car02, JM07a]. **duplexes** [BL08, NL08]. **duration** [CCSJ00]. **during** [IZA06]. **dyad** [CHRL09]. **dye** [BG00, KS05c]. **dye-sensitized** [KS05c]. **Dynamic** [SDCG02, XLZ08, CC07, CVR08, CEP07, FEV+09, JW06, mJlZyL+08, LW04a, LDG02, LEV+09, QCK01, QCK02, SDL+09, SCC04, SYC08, WM06, XLC08, YCS07, YCXY03]. **dynamical** [CKW09, EM03a, Kri09b, LDTS07, MS03, LPK07]. **dynamically** [CvG08]. **Dynamics** [BBG+04, DJB02, KB09, KIM+09, SSBE06, Yos02, ALB09, ATMK03, AM06b, BL09, BB05, BWE05, BRDC02, BSJ01, BG07, CLP09, CLC09,

CADW03, CW02, CIB05, CCSJ00, CF06, CPC⁺00, CCP04, CMD⁺04, DLG00, DSS03, DBGV07, ES00, EMP07, ESM06, FSM09, FHRR07, FG02, FBDG06, FEVM01, FKZ09, FNP⁺06, FPN⁺05, GL04a, GL04b, Gly06, GS02, GS03, Gon07, GSDT09, GJK00, HB09, HGMB04, HSWN01, HN02, HTSR04, HW03, HTN03, HLB09, Ike04, ITS05, ITS06, IC08, JS07a, JP09, JCL05, mJZsLyL07, JHZ09, KMH02, KŠB09, KM00, KM07, KSY⁺00, KAK⁺09, KZRO03, Kol04, KvGH01, KPR04, Kri08, Kri09b, Kró03, LLM08, LSG06, LPK07, LGB⁺09, LWY⁺09, LR03b, Loe03, LMIF06, LM03, LPB03, MB00, MFB04, MN02, MM03, MABM09, MBC08, MCR08, MDA08, MOP⁺07].

dynamics

[Maz01, MVL⁺05, MO09, MH08b, MCM04, MST⁺08, MS01, NK01, NBJ04, NYK⁺09, OO04, OO06, OR05, ON07, PMGL03, PRKP05, PMB04, PBW⁺05, Pin01, Pin03, PZS04, PPYS08, PHH⁺08, PHRR08, PB02, PNG08, QNF09, RRZA08, RMHK03, RG08, SO07, SH09, SBJ08, SBG⁺09a, SLL⁺04a, SM03, STH02, Ste04, SDM02, TYN05, TLKT00, TFN04, TK08, Tru07, UTH⁺03, VSK⁺04, VCM01, WCF04, WLLS04, WLL07a, WyLG⁺09, WWL⁺09, WEE01, WD08, WDX⁺02, WLL⁺03, XLL⁺02, XLZ08, YXC⁺07, YLZ08, YGLvG06, YTH⁺07, ZZL04, ZWL⁺05, ZWS⁺09, ZWZ09, ZSK07, SO07].

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

E-state [SPGS08]. **E1** [YT04]. **E2** [RY09]. **EADock** [GZM09]. **early** [CMCB08]. **earth** [JHMB⁺09, JHMB⁺11, SO07]. **earths** [LZZC09]. **ECEPP** [Sen06]. **economic** [FZL07]. **edge** [XWL⁺09]. **edge-doped** [XWL⁺09].

Edited [Sta00]. **Editor** [JW12, WM12, vLBBR12, Lip00]. **editor-in-chief** [Lip00]. **Editorial** [Bro05]. **Editors** [BFS07, FA01b, FBS09]. **educing** [BS01]. **Effect**

[CXZ⁺09, CN05, CEP07, KGL07, Mue01, WMW04, BB08, CPJ00, CPJ01, CGB⁺09, CSB08, CKT⁺08, DMJV05, GT03, HK08a, HK08b, KT08, KMM07, KCL00, Kri08, Lee09, LL01, LCDA03, Mas04, MZL08, PCS04, RY09, RR05, SOOF05, SPDS01, SCG04, SDL07, VM07, WM06, WDX⁺02, XWL⁺09, ZY01, ZZS⁺07, ZWPR⁺04, CPDZH08, HFS⁺07, JD09, WMW03, WSC09, vE01].

Effective [OCB02, SBLK01, VBGL⁺00, BCF⁺09, CR09a, DPT03, HMWC03, HSWW00, LFK05, MML02, NGTB03, NG04, RPMP03, SG07b, Vas02].

effectively [SMGE08]. **Effects** [DXW08, KKH⁺07, RLP08, XWXC08, AD00, ASS⁺02, BA03, BA04a, BA04b, BPC01, BE07, BDW00, BBI⁺09, CC07, CKF01, CDPL09, Don08, Dra00, ECA06, FGR07, FHF⁺01, GWM08, GVATG03, GM04, GGLR00, GKTS04, HRR05, IC08, JJK⁺00, JWB05, KSK00, LS08b, LR03b, Loe03, LFR⁺04, MDA08, PBF09, PSF⁺08, PWFS01, RRCA08, SF07, SL09, SMAv00, SURG06, SM06, SN06, SRB06, VDM06, WMGK07, WD04, Wib04, XYN⁺06, YXZ⁺04, YH09, ZX04, ZWS⁺02, CM09].

efficacy [KSM05]. **Efficiency**

[IO08, MKGA06, RLER04a, YAÇ⁺02, CN03, FSM09, GF08, KK08a, LJ04, LJS05, LKW04, PSMB05, SM08b, SM03, SE08, vLBBR12]. **Efficient**

[AT02, BP00, BB05, CSJ01, DMZT08, EA08, FL08, FKZ09, GHH07, GB04, HMWC03, HTKG08, KMA⁺07, KCL00, Nil09, OD09, Oos09, SATO04, SSM08, TP01b, WM12, YZ04, Ami00, BL09, BP02, BdPRMAI00, CGG06, CIB05, CY09, CY13, DBS08, FG02, GJL⁺08, JBJB00, JJB02, KM00, LSO04, LCKL05, PRSMM02, 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, ÁCD⁺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, BMLV04, BI06, BRS07, BL00, BAÁ07, CRC⁺08, CXZ⁺09, CR09a, CHRL09, CKT⁺08, DVP⁺02, DVRP⁺03, EL09, FLOD07, FR06, FS04, FZL⁺06, FSS00, KGRG08, GGA00, GR07, GBJ03, HLS07, Hir08, HSWW00, IKN08, ITN⁺05, IS07, IN01, Jac09, KS05a, KK08c, Kle03, KFD06, Kri09a, KKMS04, Lai07, LMV07, Lee09, Leh06, LV08, LL01, LLXS02, 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** [YH09]. **electron-pair** [FS04]. **electron-repulsion** [Kri09a]. **electron-sharing** [BRS07]. **electron-transfer** [QZZZ03]. **electron/four** [GYMN07]. **electronegativities** [dSGCG00]. **electronegativity** [ALC08, BCNs07, JVVK09, VK06]. **Electronic** [CWWS07, DHM⁺03, FLK⁺07, GGGLL05, Hua09a, IME02, KHY00, KMM07, KGD06, LPP06, LTF⁺07, OS08, QB05, RPNJ07, SCP08, Wu06, WWS07, XZ05, AJ03, AEE⁺03, Ama02a, AZS⁺04, AGSFA⁺05, ASS⁺02, Bac09, BBG⁺04, CMàGL⁺04, CZFH07, CN05, CNN07, CAG07, CRSB03, CSV⁺07, CTFC08, DD00, FL08, GJL⁺08, GBL⁺05, GM04, HMMS09, HZ09, Hua09b, Kar01, KRM⁺02, KJP⁺07, KIFK07, KWK⁺00, Kri09a, KPZK06, LWK08, LWLS07, LWZ09, LFR07, LB08, LDL⁺09, LMRVFH⁺09, MKGA06, MM02, NYH02, PP08b, PMC⁺08, QCK01, QCK02, RRCA08, RS05, SSB⁺03, ŠBL05, TD08, TT01, TD06, TDK07, WMRW⁺01, WLX⁺05, WL00, YXZ⁺04, YFR05, YS00, ZZY07, ZZS⁺07, ZZY08, ZXYF09, ZX08, ZL05, ZL07, ZL09b, ZM03, SMK00]. **electrons** [HIM07, Pog03, WJ00]. **electroosmotic** [YSJ09]. **electrophilicity** [RUPH06]. **electrophoresis** [WWL⁺09]. **Electrostatic** [CCT⁺03, GYMN07, PK05, PML03, RLER04b, SG07b, ABWT09, BCNs07, CPUGD09, CHMI05, DWNB01, FOL⁺04, GY06, GPK05, GBJ03, KFZ03, KLH⁺04, KCK⁺08, MMPK01, PMB04, PP08b, RLP08, SMAv00, SHSF05, VGDSU08, VC04, WCK00, YH06]. **electrostatics** [HS01, MLJ03, RSP03, STSF02, VVBV02, WMS06, ZFW08]. **electrotopological** [SPGS08]. **element** [Ara04, BHW00, BK08, BH03, BF04, HBW00, HBW01, Li01, SRB06].

elements [ABWT09, ATM⁺07, ASS⁺02, Ell07, JGH00, RP07b, RRS09, VB03, WL04, vW06]. **elevated** [TK08]. **ELF** [SFC04, CFS03, FSS00, PC05, PC07]. **ELI** [BWW⁺08]. **ELIA** [BWW⁺08].
elimination [Adc04, CFD03, GLD08, GS08, KUB07, Mui05, PSDM00, YFS07].
Elongation [KLM⁺09, MKGA06]. **Elucidating** [DBS07]. **elucidation** [GZ07, GLH⁺08]. **embedded** [CEP07, GGLR00]. **embedding** [Agr03, JNV08, KS02b]. **emission** [MLCD01, RGG08]. **emitting** [LFR07].
Empirical [CBC⁺08, LS08c, Mac04, SP05, CYM02, FM00, Gri04, GGK⁺08, HRBKB03, JČHS07, KK08b, LR03a, LLM09, MB00, RKH03, ZNLL07, VBGL⁺00].
employing [MHT01, THHN01]. **empty** [CZA03]. **enantiomerization** [Qua07]. **encapsulated** [WL09b]. **enclose** [ZBS03]. **Encyclopedia** [vRS98, Lip00]. **end** [Adc04, GLD08, KUB07, PSDM00, YFS07]. **endohedral** [KSN01]. **endoperoxide** [BLO⁺02, CG08]. **enediyne** [KC01a]. **Energetic** [DRAS04, DRAS05, JW12, RP09, BCP03, ECM⁺03, JD09, KCK⁺08, 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, DMZT08, FOL⁺04, FJP07, FKU⁺05, GS04, GKTS04, HT05, HYA02, Hol05, IO08, JJK⁺00, JCL05, JZD⁺09, JG03, JSHG07, JČHS07, KWK⁺01, KWK⁺02, KSTC01, KC01b, LN01, LSW⁺01, LFEdL06, MT03, Mas04, MLL⁺08b, NHH05, PK05, PSF⁺08, RSSKB03, RSE07, RSN⁺02, RM00, SZT08, STSF02, SYC03, SA07, SLRC01, TKS⁺01, UBDPJ04, Var09, VC04, WCK00, WLX⁺05, WS05b, WW04, XLT07, ZMZ09, ZW09, ZM03, vGGB00].
Energy [CBH⁺03, HFHL06, IN08, KLS02, MSF⁺08, NK06, SSB07, WM12, dSR08, AMR04, AJ03, ABÅ04, AE06, AM06b, ABBC01a, ABBC01b, AGSFAL05, BM07, BCIB05, Ber03, BL05, Blo04, Bof01, BRLS08, BRLS12, BACJCT01, BF07, BLB09, CC09, CN03, CCB04, CY09, CY13, CJW⁺09, Chi03, yCkHmY08, CV09, CMGDAC⁺07, CA04, COL⁺06, DLD⁺02, DLRZ09, DMJV05, DK01, EGSG00, FSM09, FK07a, FKJ⁺01, FZL⁺06, GZL02, GMA04, GLMV09, GAdGM08, GG09, GC04, GS02, GS03, GPSP06, GB02, GWS⁺02, HKMS01, HP01, HR08, HMOG07, IGNH03, ILKR09, IGL07, IPN06, IPN07, Jac09, JMD⁺02, KGN07, KN04, KKC05, KUB07, KB09, Kob03, KC01b, Kri09a, Lab08, LR03a, LMK01, LF04, LFZS04, LJ04, LBG08, LKW04, Lu09, MG06, MCF05, MAF⁺07, Maz08, MH09, MGJAARC00, MGLO03, MRS⁺07, Nak02, NKIS02, NA06]. **energy** [OD09, OFB08, ONHN00, OKH⁺02, OV03, Oos09, PSC⁺01, PMGL03, PK04, PAT⁺09, PMPGP05, Qua01, RP07a, Rao00b, Rap06, RSE07, RRCA08, 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, OO06, SM08b, SM03].
ensembles [GLD08, Ike04]. **ensure** [FKFG08]. **enterovirus** [KCL06].
Enthalpies [EB04, WC04, BE06, LS05b, RM00, TTBM09, VGGMM05].
enthalpy [OVMV04]. **entire** [ZAT07]. **entropic** [CBC⁺08, FGR07].
entropy [DHF⁺05, HDF⁺07, HTKG08, KKH⁺07, LM03, RK05, 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** [MPF00, ZFW08]. **enzymatic**
 [PCMG09]. **enzyme**
 [CFER04, Fie02, GGLR00, GS04, MDA08, Pin03, TDH06, VB09, ZL09a].
enzymes [BS06, CPUGD09]. **enzymic** [CG05, TCR⁺02]. **Epimerization**
 [BBSS06]. **Epitope** [SHBD05]. **epitopes** [KVS⁺06, SHBD05]. **epoxide**
 [Owe05]. **epoxides** [OY01]. **epoxy** [OY03]. **epoxy-amine** [OY03]. **EPR**
 [SN06]. **equalization** [BCNs07, JVVK09, VK06]. **equation**
 [AMR04, ABWT09, BHW00, BH03, BF04, BF07, BRS00, BRS01, FS00b,
 Höf05, HBW00, HBW01, SATO04, TW03, Vas02, Vis02, Zho06]. **equations**
 [Bie04a, CF04, DOSG06, Har04, KvGH01, LPK07, LMJ02, QNF09, RI07,
 Rud05a, Rud05b, Rud05c]. **equilibrated** [CA07a]. **Equilibration** [SDCG02].
Equilibration-Morse [SDCG02]. **equilibria** [FGR07]. **equilibrical** [Kli01].
Equilibrium [KSTC01, BBP09, ECA06, KBLP09, LS08b, MMLC05, PAS08,
 ST04, WMGK07]. **EQUIPATH** [Kli01]. **Equivalent**
 [ZZY07, WBSR03, ZZY08]. **equivalents** [RCJ02a, RM00]. **ERE** [MCF07].
Erratum [ABBC01a, Ano05b, Ano06a, Ano06b, Ano06c, BA04a, BRLS12,
 CY13, FS00a, HNWF12, HBW01, HK08a, JHMB⁺11, KWK⁺02, LFSB03a,
 LR03b, NBTN04a, PCO⁺07a, PWHF⁺04, RS07a, TZX01b, WB04a, WB05,
 WMW04, WWC⁺05]. **error** [IO08, KMA⁺07, Kob03, Mas04, MDI04, RS05,
 Rud05a, Rud05b, Rud05c, TBSM09, VKP⁺08]. **error-ranked** [TBSM09].
errors [CS03]. **erythronic** [vDSSvA04]. **ESFF** [SYY⁺03]. **Essay**
 [BHTCG07, FK07b, GR07, Kut07, MGCA07, Nye07, Sha07, Sim07, Tru07].
established [SB01]. **ester** [TH02]. **esters** [POJ01]. **estimate**
 [KC01b, YZ04]. **estimated** [ZMZ09]. **estimates**
 [GC04, HT05, MDI04, SY09]. **estimating** [HDF⁺07]. **Estimation**
 [DHF⁺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**
 [ACLD03, LCDA03, LCGA03, LCA03, ZWY⁺09]. **ethyl** [KKH⁺07].
Ethylene [TBG00, BSJ01, Hir08, NTH00, SBB02]. **Euclidean** [RRS09].

EUDOC [PPXP01]. **Euler** [SG01]. **evaluate**
 [GGB07a, GGB07b, LF04, OSHS03, TSSGS07]. **evaluated**
 [ABBC01a, ABBC01b, Bof01, 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, KJVW08, KH06, LMV07,
 LYS08, MSH⁺06a, Mor02, PRS04, Sha05, VP02, WL02, Yan04, Yas08,
 CBC⁺08, GKTS04, OGH05, ZSK07]. **evaluations** [SF05]. **Evans** [SRK⁺00].
EVEBAT [CZA03]. **Even** [CVVB04, CC07, VVBV02]. **Even-tempered**
 [CVVB04]. **evidence** [BLO⁺02, IO08, SFR07]. **Evolution**
 [SPL⁺02, Der09, Mck07a]. **Evolutionary**
 [DPRR05, CS02, CKR08, yCkHmY08, DB06, KH05, VGO⁺07, YK00, Yan04].
Ewald [Ami00, BYQS03, KM00, KSY⁺00]. **Exact**
 [GC02, GHMP03, DLSVY00, TRS02]. **examination**
 [CZA03, LJKL08, QNF09, WL04, ABÅ04]. **example**
 [AS00, JHPRSM⁺05, MGLL03]. **examples**
 [CMA⁺08, HBW00, HBW01, SDL⁺09]. **exchange**
 [AAP00, AKN07, BWI⁺02, EL09, FSM09, FGR07, FDM00, GLP08, LMIF06,
 RRFC⁺03, SM08a, SM08b, WL04, Wei08, NCO⁺05]. **exchange-correlation**
 [AAP00, EL09, FDM00, WL04]. **Excitation**
 [HKHN08, BMB07, Che01, CG08, Hol05, LWZ09, LFEdL06, ON07, PSF⁺08,
 SZT08, SA07, SLRC01, XZ04, ZM03, vGGB00]. **excitations**
 [DHM⁺03, ION07, MA09, TJM⁺03, XZ05, ZX04]. **Excited**
 [CHA⁺07, HFS⁺07, Ang09, FCW06, FDSA00, HNWF07, HNWF12, IR03,
 LWX07, LDL⁺09, MW09, NBTN04a, NBTN04b, NTH09, PO03, PSS⁺04,
 SBI08, SMKM00, TY03, TKN⁺08, WLZ⁺07, ZH08]. **excited-state**
 [LDL⁺09, NTH09, PSS⁺04]. **exclusively** [RI08]. **exercise** [FLK⁺07]. **exist**
 [RY09]. **existence** [WPH⁺07]. **expanding** [Bac07, Bie04a, IZA06].
expansion [AHGK09, GS09, GKH05, HTKG08, II02, Ish02, LZZC09,
 SvDS01, WBSR03, ZFL⁺05]. **expansions**
 [Bou01, DWNB01, GC02, JSHG07, RLER04b, SG01]. **experiment**
 [BE09, GBJ03, LS05b, Mat03]. **experimental** [BE06, JARM02, LEK07].
experimentally [KBN02, TDH06]. **experiments**
 [CVR08, HP05, OD09, PC00, PFC03, SL04]. **Explicit**
 [EC06, PPYS08, RI07, AL01, DMJV05, FC06, HM02, JZD⁺09, KIFK07,
 KIM⁺09, LSO04, PK05, RKA⁺09, WB04a, WB04b, WB05, ZGFL01].
explicit/implicit [LSO04]. **exploiting** [JSHG07]. **exploration**
 [CSJ01, HLB09, LXW⁺09, LMO09]. **exploratory** [PGH⁺04]. **explore**
 [ILKR09]. **Explorer** [SHBD05]. **Exploring**
 [BL05, HPP00, HXLS09, KF08, Sch03, Tie09, SPL⁺02]. **exponent**
 [WTKM06]. **exponential** [Rud05a, Rud05b, Rud05c]. **exponentially**
 [Bie04a]. **exponents** [MY08b]. **exposure** [MML02]. **expression** [dGWH01].
expressions [TNS00]. **Extended**
 [LMH⁺09, TVL⁺03, Bie04b, Cul04, DXW08, KUB07, QNF09, SS00, ST01].

Extending [GCD04, MFB04]. **extensible** [SYY⁺03, GBL⁺05]. **Extension** [CR09b, FBLO08, GY08, TBGRJ04]. **Extensive** [JW12, LB08, SLHW09, YXL⁺09, ZL05, SMG09]. **external** [CM09, EC06]. **extra** [LW07]. **extra-valence** [LW07]. **Extracting** [HM02]. **extraction** [OD09]. **extrapolated** [KSTC01, Var09]. **extrapolation** [MO09, MC06, PSC⁺01, PFJ⁺03]. **extremal** [ZZ08]. **extremely** [GFS05]. **Eyring** [Nye07].

F

[CRC⁺08, FO04, Gog08, HYA02, HZ09, Hua09a, IV04, KS05a, KBL08, Mar03, RB01, STC⁺08, UTT⁺04, WLLS04, WLL07a, XLL⁺02, ZY01, ZLLS06b, ZL09b, HK07, KS05a, RFSS06, SOOF05, Sha02, WDWS06, YWHZ03]. **facility** [SWZS04]. **factor** [LMCD09, WL00, XSHC06]. **factorization** [EC06]. **factors** [AST06, SBH02, TP01b]. **FACTS** [HC08]. **family** [CFS⁺09, DMC05, NAT07, WTKM06]. **FapydG** [SHD⁺08]. **farnesyl** [SFR07]. **Fast** [JBJB00, JJB02, JSHG07, NG04, RS08, SYC03, SFC04, Ami00, ATMK03, Ano05b, CS02, CRG01, CHMI05, CZA03, GY08, GKK07, HH04, HLM05, Ish04, KM00, KLM⁺09, KvGH01, KH06, PZS04, RK05, San01, SCC04, Sha05, TRS02, VP02, WCC08, HC08, LZ05a, VLH⁺05]. **faster** [SF05, AM06a]. **faujasite** [TLOG00]. **faujasite-type** [TLOG00]. **FB** [DHW⁺09]. **FB-QSAR** [DHW⁺09]. **FBP28WW** [PAT⁺09]. **FDS** [TJE03]. **Fe** [BTP09, HLLN06, HYR06, KRLD09, AGK03, KT08, DF04, Mck07a, Mck07b, NyHN06, NHN06, PLC08]. **feasibility** [MWE02]. **feed** [SJJ⁺04]. **feed-forward** [SJJ⁺04]. **feedforward** [LJZ⁺07]. **Felix** [Ano06a, Ano06a]. **FeMo** [Mck07a, Mck07b]. **Fermi** [Kri09a, PYCD03, PYS05, PC07, PLC08]. **ferrocene** [Kan07, MBP09, ZZS⁺07]. **ferromagnet** [TD08]. **ferromagnetism** [SK08]. **FeS** [Mck07a]. **Feynman** [RLER07]. **Field** [MO01, AS06, ACLD03, Ano06b, Ano06c, ATBLS04, BWI⁺02, CLP09, CLWL09, CPM03, CM09, CGB03, CLA⁺00, CR02, CSU05, DvG00, DPT03, DRMD03, DFWH05, DMLI05, DGI⁺08, DHW⁺08, DWC⁺03, EBD⁺01, FHRR07, FBDG06, FAR02, FM00, GZL02, GMA04, GRO⁺03, GGK⁺08, HP01, HGMB04, HXLS09, HIM07, HNL08, HMOG07, IDMC09, IT03, IKYM09, JS07b, JCL05, JM07b, JFG04, KB02, KSB⁺02, KS06, Kar06, KFNH08, KTA03, KOFF09, KLB03, KYT⁺08, KOML08, KDSV02, KVL⁺04, KBN02, LL00, LST08, LTV08, LFZS04, LAT05, LH05, LLM09, MT03, MB00, MM05, MP03b, MBC08, MMMY07, MSR04, MRC03, MHJS06, NUH02, NCO⁺05, OYH05, OMNH08, ONHN00, OKH⁺02, OVMV04, OBT09, PB04, PMB04, PS09b, PWHF⁺03, PWHF⁺04, Pom04, PHH⁺08, POJ01, PB05, RSN⁺02, RKH03, SF07, SO09, SDL⁺09, SDvG01, SAS05]. **field** [SDCG02, SSS⁺09, SYY⁺03, SHK⁺05, SP05, SK05, TAS07, TTB01a, VSW⁺03, VCM01, VTT⁺08, WK01, WWC⁺04, WWC⁺05, WZW⁺06, WMS06, Wil01a, Wil01b, XLT07, YCXY03, ZWC⁺09, vDSSvA04]. **field-based** [DMLI05]. **field-derived** [WMS06]. **field-induced** [CGB03]. **fields** [ABÅ04, Car02, EBD⁺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, Bie04b, BF04, DRMD03, Der09, GM04, HBW00, HBW01, KGD06, PZS04, RP07b, Rud05a, Rud05b, Rud05c, VZM⁺08]. **finite-chain** [Der09]. **finite-difference** [Bie04a, Bie04b, Rud05a, Rud05b, Rud05c, VZM⁺08]. **finite-temperature** [KGD06]. **fire** [LDC⁺07]. **First** [CS01, HZX04, Hua09b, TK08, WZZ⁺09, WD08, ZDS⁺05, ZXYF09, ZHMW09, AD00, BP03, CJK⁺02, EBL⁺08, FO08, GJL⁺08, GD09, JPCA08, KK08c, LWZ09, LK03, Mck07b, 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, ZXYF09, EBL⁺08, GD09, WLX⁺05]. **first-row** [AD00, BP03, LK03]. **fit** [BCNs07, SY09]. **fitted** [YOB⁺08]. **Fitting** [KC01b, MCF05, Wei08]. **five** [SBH02, Van02a]. **five-coordinated** [SBH02]. **fixed** [HM06]. **fixed-composition** [HM06]. **Flex** [GCD04]. **flexibility** [BL08, BCP04, KG02, KTA03, MHL⁺09, OV03]. **Flexible** [COS01, NGTB03, YK00, AGI⁺00, AGI⁺07, AJ03, AHGK09, BZP09, BTLP03, BS08, CCL06, CKMC04, CLH⁺07, DDKV07, GCD04, HW09, JNV08, KOFF09, MH08b, SSBE06, TFN04, TP01a, Tot04, VLH⁺05, vEMK01, vE01, TJE03]. **flexible-backbone** [AHGK09]. **flexible-ligand** [HW09]. **flexible-protein** [HW09]. **Flooding** [LSG06]. **Fluctuating** [OR05, KMH02, PB04, PMB04, Yos02]. **Fluctuation** [MHW04, 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]. **fluoride** [BSG07, IV04]. **fluorides** [KS05a]. **fluorinated** [CUSS03]. **fluorobenzene** [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, AKN07, Bou00, Cul04, DD00, GAdGM08, HDBD04, MS00, MBWP03, PFJ⁺03, PVdJB00, TYO⁺02, UIHN09, WMW03, Wei08, YH07, vDSSvA04]. **Fock/Kohn** [RRS07]. **Focus** [Mat03]. **focusing** [KBK⁺01]. **fold** [DB06, ZM06]. **folded** [CP08, GB04]. **Folding** [HEP⁺02, ADM⁺06, CCC03, DvG00, HG08, IM06, JS07a, JIK09, KH05, MLG04, MH09, Mei02, MWE02, RSER09, RLP08, VW00, VW04, VGO⁺07, ZP03, dSR08]. **folds** [BS01, ZS04]. **following** [DLD⁺02, LMO09]. **For-Gly-NH** [PC00]. **For-L-Ala-NH** [PC00]. **Force** [CLP09, JCL05, OMNH08, OBT09, SO09, SL09, ZWC⁺09, AM07, AS06, ACLD03, ABÅ04, Ano06b, Ano06c, ATBLS04, CLWL09, Car02, CPM03, CLA⁺00, CR02, CSU05, DvG00, DGI⁺08, DWC⁺03, EBD⁺01, FBDG06, FAR02, FM00, GRO⁺03, GGK⁺08, HP01,

HGMB04, HXLS09, HRBKB03, HFSD03, HNL08, HMOG07, IDMC09, IT03, IKYM09, JS07b, JM07b, KB02, KSB⁺⁰², KS06, KFNH08, KTA03, KOFF09, KLB03, KYT⁺⁰⁸, Kle03, KOML08, KDSV02, KVL⁺⁰⁴, KBN02, LLM08, LL00, LMGO⁺⁰⁹, LHI09, LAT05, LH05, LLM09, MT03, MB00, MM05, Mac04, MFB04, MMLC05, MBC08, MMY07, MSR04, MRC03, MHJS06, NCO⁺⁰⁵, NMAT01, OYH05, OSHS03, ONHN00, OKH⁺⁰², OVMV04, PB04, PMB04, PK04, PS09b, PHH⁺⁰⁸, POJ01, PB02, PB05, RP07a, RNG03, RI07, RG08, RKH03, SDL⁺⁰⁹, SDvG01, SAS05, SDCG02, SF05, SSS⁺⁰⁹]. **force** [SY⁺⁰³, SHK⁺⁰⁵, SP05, SMM⁺⁰⁸, SK05, TAS07, TTB01a, VSW⁺⁰³, VCM01, VTT⁺⁰⁸, WK01, WWC⁺⁰⁴, WWC⁺⁰⁵, WZW⁺⁰⁶, Wil01a, Wil01b, XLT07]. **Force-field** [CLP09, OBT09, SO09, HGMB04, IDMC09, KLB03, MBC08, NCO⁺⁰⁵, OKH⁺⁰², OVMV04, SP05, VCM01]. **forced** [CAG07, LPB03]. **forcefield** [Adc04]. **forces** [BCF⁺⁰⁹, BH03, HNWF07, HNWF12, JS07a, LPB03, PK05, RLP08, WB04a, WB04b, WB05]. **Foreword** [DF08, Fre00, FJ02, FH06, FS07, Gad03]. **form** [AT02, Bac07, BRS01, CR02, LC07]. **formaldehyde** [WCL05]. **formalism** [AS00, FLGW00, YCXY03]. **formalisms** [CF06]. **formamide** [IINK09, Pac06]. **formamidine** [WJX⁺⁰⁸]. **format** [TDK07]. **Formate** [ČJPZS08, NK06]. **Formate-Lyase** [ČJPZS08]. **formates** [CUSS03]. **Formation** [JM07a, RAGLL09a, RAGLL09b, BE06, BMTFR08, CS03, EB04, HIA03, JWB05, Kle02, LLA01c, LYZ⁺⁰⁸, Nee03, RCJ02a, RM00, TT08, TTBM09, WC04, WX09, ZZW09, dOMSL01, JKM08]. **formed** [LLW02, LSW⁺⁰¹]. **formic** [Pac06]. **forming** [PP08a]. **forms** [SPT07]. **formulas** [Ish02, Tor02]. **formulation** [BF07, Cul08, PK05]. **formyl** [GSB09, HJCP01, PFC03]. **formylglycinamide** [HRBKB03]. **forward** [KM07, SJJ⁺⁰⁴]. **Four** [SH02, FJ08, GPSP06, Lai07, PVdJB00, PV03, SBH02]. **four-** [Lai07, SBH02]. **four-centers** [GYMN07]. **Four-component** [SH02, GPSP06, PVdJB00, PV03]. **four-index** [PVdJB00]. **four-membered** [FJ08]. **Fourier** [BWP07, CGG06, HLM05, TYN05]. **fourth** [Bie04a, Rud05a, Rud05b, Rud05c]. **fourth-order** [Bie04a, Rud05a, Rud05b, Rud05c]. **FPT** [BPC01]. **fractal** [Pan07, TT08, XOW⁺⁰⁰]. **fractional** [MGLO03, SM08b]. **fragilis** [SDM02]. **Fragment** [DHW⁺⁰⁹, CFK08, DPM09, FOK⁺⁰⁴, FKL⁺⁰⁶, FII⁺⁰⁷, FKU⁺⁰⁵, FKM⁺⁰⁶, FKM⁺⁰⁷, IIK09, KIFK07, MLG04, MLL08a, NYK⁺⁰⁹, NGTB03, NG04, OO08, SG07b, ZMZ09, KIM⁺⁰⁹]. **Fragment-based** [DHW⁺⁰⁹]. **fragmental** [CSB⁺⁰³]. **fragmentation** [Gor01]. **fragments** [AM09, DWNB01, DPRR05, KS01a, LV08, NG04, PBF07]. **Framework** [JGVF05, CR08, EA08, FS04, TAS07, Tie09]. **Framework-based** [JGVF05]. **Franck** [Ama02a, LMCD09, TP01b]. **Free** [DLRZ09, GS03, JMD⁺⁰², MH09, PMGL03, YXC⁺⁰⁷, AM06b, BG00, BWE05, BLL⁺⁰⁶, BCIB05, Blo04, CN03, CM09, CY09, CY13, Chi03, CV09, CCK01, CMGDAC⁺⁰⁷, CG05, COL⁺⁰⁶, DMJV05, FSM09, GZL02, GMA04, GLMV09, GG09, GC04, GS02, Gra07, GWS⁺⁰², HKMS01, HR08, HMOG07,

ILKR09, IGL07, JZD⁺⁰⁹, KDG⁺⁰⁹, KAS⁺⁰⁷, KKC05, KUB07, KB09, Kob03, KK01a, Lab08, LR03a, LF04, LSW⁺⁰¹, LKW04, MG06, MT03, MGLO03, MRS⁺⁰⁷, OD09, ONHN00, OKH⁺⁰², OV03, OVMV04, Oos09, PK04, PAT⁺⁰⁹, RSE07, RWBH09, SOOF05, SAM06, SKGS00, STSF02, ŠBL05, SSM08, SY09, UBDPJ04, UTH⁺⁰³, VLH⁺⁰⁵, VE09, VGDSU08, VM02, WHF08, XLT07, YZ04, ZMZ09]. **free-base** [ŠBL05]. **Free-energy** [JMD⁺⁰², AM06b, CY09, GMA04, ONHN00, RWBH09, SKGS00]. **Free-energy-driven** [MH09]. **freedom** [DHF⁺⁰⁵, MZL08]. **freeze** [BME05]. **freeze-and-cut** [BME05]. **frequencies** [BRV⁺⁰⁷, Han01, Kle03, KBN02, LMB08, PZWG⁺⁰⁴, WM04, ZWPR⁺⁰⁴]. **frequency** [DF06, DR09, MY08a, VSW⁺⁰³, YH07]. **frequency-dependent** [MY08a, YH07]. **friction** [JS07a]. **frozen** [AEE⁺⁰³, GWS⁺⁰², JNV08]. **fructose** [MRS⁺⁰⁷]. **fuel** [CCCJ09]. **Fujitsu** [KSY⁺⁰⁰]. **Fukui** [DVP⁺⁰², FS04, TSSGS07]. **fulfillment** [RLER07]. **Full** [PRSMV08, GD09, IR03, KGD06, RS08, ZCZ03]. **full-atom** [RS08]. **fullerene** [CHRL09, CTFC08, GYCZ04, GXK09, Kan07]. **fullerene-dizincocene** [GXX09]. **fullerenes** [GZ07, GM01]. **Fully** [GWM⁺⁰⁰, XZZ04, WTKM06]. **function** [Bac04, BS05, BdPRMAI00, CFS⁺⁰⁹, Che01, yCkHmY08, CPUGD09, Con02, DMZT08, DP03, FSS00, GCB03, GS09, GdAcV⁺⁰⁷, GPN01, HMWC03, HZ06a, HZ06b, ILB03, ILKR09, Ish04, KK08c, Kni00, KFD06, LR03a, LHI09, LBT07, MP03a, MML02, MY08b, Nak07, NKIS02, PP08b, PA05, PAS07, SFC04, SJW09, TLKT00, TW03, TJE03, TT05, TSSGS07, VVS07, YLL⁺⁰⁹]. **functional** [AAP00, AB00, ABYM08, ASY01, Bac09, BP01, BE09, CLP⁺⁰⁵, CFK08, CRS05, CR08, CSB08, CPML08a, Cul04, DVRP⁺⁰³, ECM⁺⁰³, EL09, FCW06, FZL07, FG02, GHLK⁺⁰², GM01, GLRL02, Gri04, Gri06, GBBH09, Haf08, Han01, HNWF07, HNWF12, Hol05, ION07, IB04, ITN⁺⁰⁵, IS07, JFG04, JČHS07, KGL07, KSS08, KWK⁺⁰¹, KWK⁺⁰², KZW⁺⁰⁵, Kri09a, LRI⁺⁰², LWK08, LMB08, LMGR05, LLS03, LWH06, LKT04, LF02, LLZL09, LDL⁺⁰⁹, LZF⁺⁰⁹, MW09, MSBS01, MW00, NTH09, NAT07, OKE⁺⁰², PSF⁺⁰⁸, PU09, PDS01, QZZZ03, QZL⁺⁰⁴, RB01, RK04, RDM⁺⁰⁸, RR05, RZWS07, SH07, SZT08, SPT⁺⁰³, SPT07, SLRC01, SSB07, SW06, TBG00, TST⁺⁰⁸, TKN⁺⁰⁸, TKH03, Van02b, VMA03, VL00, VBS09, WRP⁺⁰⁶, WB07, WZY04, WMRW⁺⁰¹, WL02, WCW08, WCHW09, WM04, WSC09, WCL05, WZXY07, WM01, XYN⁺⁰⁶, XB08, XWC09, XL02]. **functional** [XPW09, YYW07, YLL⁺⁰⁹, ZZL04, ZH08, Zho06, ZM03, vGGB00]. **functional/continuum** [LRI⁺⁰²]. **functionals** [BP03, DF04, Han01, ION07, JPCA08, KRM⁺⁰², KS01b, PJPJdPRMI07, SCF⁺⁰⁹, WL04, YTH01]. **functions** [AE06, Bac07, Bou00, CGB03, CGSdST06, DVP⁺⁰², GFS05, GLD08, GS07, GBJ03, IT03, MLL06, MY08a, NUH02, OFB08, PFB05, RHL09, Ruv07, SS00, TS05, TD06, WG02, YH06, ZM03]. **Fundamental** [LMB08]. **fungal** [LPP06]. **funnels** [HEP⁺⁰²]. **furfural** [COMR⁺⁰⁴]. **Further** [GPK05]. **fusion** [CRGN07]. **fuzzy** [ALTB06, EKB02a, RLA01]. **FVII** [PDP02].

G [AGI⁺07, Kr603, XWC09]. **G**** [Wib04]. **G-protein** [XWC09]. **G**. [CSD05, Sim07]. **G2** [RY09, ZKZ⁺07]. **GA** [HSMT04, HSMT04, LLL⁺08]. **GA-MLR** [HSMT04, LLL⁺08]. **gadolinium** [AB00]. **gain** [HP05]. **gains** [NYTH09]. **galabiose** [RSSKB03]. **galactose** [RSSKB03]. **GAMESS** [UKNS01, UKN04]. **gamma** [Ish04]. **gap** [KUB07]. **gap-free** [KUB07]. **Gas** [BAL⁺01, POJ01, CPJ00, CPJ01, DR09, EGSG00, JJK⁺00, JHZ09, KSB⁺02, KT08, KKH⁺07, LRI⁺02, Lee09, LZA02, LB05, LXS08, MFB04, Mas01a, Mas01b, MM02, Pan07, PV07, wQZsLyZ02, RRS06, ROG00, SMGE08, STSF02, SMK00, SK05, TDH06, UCT⁺03, UNM⁺01, WD04, XKKL03, XKG⁺05, YQQH09]. **Gas-phase** [BAL⁺01, POJ01, JHZ09, KKH⁺07, Lee09, MFB04, wQZsLyZ02, TDH06, UCT⁺03, XKKL03, YQQH09]. **Gaseous** [WDWS06, PG01]. **gases** [SRB06]. **gauge** [Ish03]. **gauge-including** [Ish03]. **Gauss** [DBS08]. **Gaussian** [TdMSD⁺08, CMJ08, Duk01, EDW07, GC02, HdMdS05, HdS06, HD06, IO08, Leh06, Lu09, MV06, MY08a, RC04, TW03, WTKM06, YJF06]. **Gaussian-2** [RC04]. **Gaussian-4** [Lu09]. **Gaussian-type** [Leh06, MY08a, TW03]. **GAUSSIAN94** [Kli01]. **GB** [GC04, WHF08, GWS⁺02, YJF06]. **GB/SA** [GWS⁺02]. **GBR** [FPG⁺06]. **GDDI** [FOK⁺04]. **Ge** [LLXS02, WDXS06, CJS⁺03, LLXS02]. **GeD** [WDX⁺02]. **GeH** [LLXS02]. **gemcitabine** [PFR04a]. **geminal** [TT05]. **geminals** [TT01]. **general** [AM07, BRS01, DGI⁺08, EBD⁺01, JM07b, KSU03, KBT03, NUH02, RG08, SAM06, TZX01b, TZX01a, WWC⁺04, WWC⁺05, XYN⁺06, BRS07, EA08, FLGW00]. **generalizable** [KYT⁺08]. **Generalized** [ADM⁺06, ILB03, AB08, BC06, Bud07, CPJ00, CF06, Cul08, DLG00, FOL⁺04, FL08, FC06, GZL02, ION07, Lab08, LFSB03a, LFSB03b, MTE04, MCM04, OCB02, SHH07, Tot04, XL02, YH07, YJF06, ZGFL01, dGWH01, BPCD07, FOK⁺04]. **generate** [BWI⁺02, CA07a, BAH⁺02]. **generated** [Kri09a, LAR⁺03]. **generating** [AMR04, CA04]. **Generation** [RLER07, BSOB05, BAH⁺02, Ell07, EKB02a, JBJB00, JJB02, KSB⁺02, LS08b, MM03, PVdJB00, PABK03, YJF06]. **generator** [Fau01, HDBD04, LN01, VW00]. **generic** [yCkHmY08, Yan04]. **Genetic** [LSY02, MM07, YL06, BMTSC01, CKMC04, HHJ03, HWDB03, HMSM06, KOFF09, LJS05, SPT07, SBH02, TP01a, WK01]. **Geometric** [CSRST04, ZZTS09, Est07, LDL⁺09, RSN⁺02, ZXY08]. **geometrical** [GRCD01, Kle03, MLL⁺08b, PJB⁺07, SCF⁺09, GCD04]. **geometries** [BB08, Han01, IZA06, JČHS07, KKY01, KJP⁺07, WB07, Wib04]. **Geometry** [Bud07, LHP01, RK04, VMF⁺03, BP00, Bie04a, BM00, Cri04, GPSP06, HHH00, IZA06, KKG⁺09, KHF⁺09, Kle03, LJ04, MBP09, MW00, PO03, Pul05, RON02, SCP08, WPS02, ZZS⁺07]. **GEPOL** [PTC01]. **Germanium** [LLXS02]. **GFP** [HFS⁺07, NINAT⁺07]. **GGA** [DDBP09, Gri06, RLDI09]. **GGA-type** [Gri06]. **GIAO** [FO04]. **Gibbs** [EGSG00, HR08, IGL07, Lu09, SM08b]. **Gilbert** [GR07]. **Gillespie** [RMP01]. **give** [JJK⁺00]. **glasses** [NA06]. **Global** [CZB07, FTLV01, JHZ09, CS02, CMBC08, LS05a, RUPH06, SE08, TSSGS07, TSSSG08, WS02a, WG02, UKN04]. **Globally** [PAS08, SPT07]. **Glu441**

[PCS04]. **glucans** [CMD⁺04]. **glutamate** [FTLV01]. **glutamic** [ZZY07]. **glutamine** [WC08]. **Gly** [PC00, VKP⁺08]. **GLYCAM06** [KYT⁺08, SDL⁺09]. **glycinamide** [LB05]. **glycine** [BA03, BA04a, BA04b, GAIMVB01, GSB09, GKTS04, KAS⁺07, LB05, LSW⁺01, MOP⁺07, PG01, ROG00, ZW09]. **glycol** [Pin01, RR05]. **glycol-lesioned** [Pin01]. **glycosidase** [BMTFR08]. **glycosidase-inhibitor** [BMTFR08]. **glycosidase-substrate** [BMTFR08]. **glycosidic** [SO09, SDL⁺09]. **glycyl** [KOML08]. **going** [CCK01]. **gold** [BR04, CZ05]. **gold-capped** [CZ05]. **GoIP** [IDMC09]. **good** [VGGMM05]. **GPCR** [XWC09]. **GPCR-CA** [XWC09]. **GPU** [NYTH09]. **Gradient** [SE07, DLD⁺02, DSR⁺07, FRLN09, GMA04, ION07, Ish02, IPN07, LST08, TNS00, WL02]. **gradient-based** [FRLN09]. **Gradients** [WM12, BWP07, HHS⁺05, IK00, KBT03, LJ04, SSMW09, vLBBR12]. **grain** [PSHP08]. **grained** [CP09, DR07, DJB02, HXLS09, MBC08, SBJ08, VSK⁺04, VTT⁺08, WWL⁺09]. **graining** [CA07a, EBAN07]. **grand** [EMP07]. **GRAPE** [Höf05]. **graph** [CLZX09, MGMM07a, Pog03]. **graphene** [KK08c]. **Graphical** [LD05b, DPDG05, JKII08, KMH02, KBT03, LW04b, LXZ06, Pra01, YNW05, hYDN⁺08]. **graphically** [GS09]. **graphics** [FEV⁺09, SPF⁺07, Yas08]. **graphite** [BCF⁺09, EKO⁺01]. **Gravitational** [WS02a]. **greedy** [TGD05]. **green** [DHM⁺03, XZ05, KK08c, KFD06, ZM03]. **grey** [XLC08]. **grid** [ALB09, CG06, Pom04, RSN⁺02, RKA⁺09, SKSH07, STH02, WL00, WRBV03, YK08]. **grid-based** [ALB09, RSN⁺02, RKA⁺09, SKSH07, WL00, WRBV03]. **GridMAT** [ALB09]. **GridMAT-MD** [ALB09]. **grids** [Bie04a, SFC04, THHN01]. **GROMACS** [KVF⁺07, LSG06, VLH⁺05]. **GROMOS** [CLWL09, CHB⁺05, LH05, OVMV04, SHK⁺05]. **GROMOS05** [CHB⁺05]. **GROMOS96** [SDvG01]. **groove** [BCP03]. **grossular** [ZWTP⁺08]. **Ground** [HM01, PO03, PSS⁺04, BBI⁺09, CWY09, FCW06, FDSA00, IR03, Kri09a, LMK01, ZOJ⁺06]. **Ground-** [PSS⁺04]. **Ground-state** [HM01, Kri09a, LMK01, ZOJ⁺06]. **group** [ATBLS04, CQ04, DVRP⁺03, Eli07, EB04, JWB05, JGH00, KBT03, LW07, MBM⁺00, MA05, RCJ02a, RZWS07, RKH03, SGPS09, SN00, TD06, dSGCG00]. **groups** [BE09, EB04, FJ08, Van02a, WSC09]. **growing** [Qua07]. **grown** [WHH⁺06]. **Growth** [TDK07, HMK02]. **Grubbs** [YXC⁺07]. **Grubbs-** [YXC⁺07]. **GS** [MH09]. **GS-** [MH09]. **GTO** [CGB03, RLRE01]. **guanine** [EL07, GWL07, HHWG08, JM07a, KKMMS04, MSBS01, MHS05, SMK00]. **guanine-** [MHS05]. **guanine-cytosine** [KKMMS04]. **guess** [Qua07]. **guest** [LMMW04, Oos09]. **GUI** [JKII08, SD09]. **Guide** [SH08, Woo01, You11, Bic09]. **guideline** [MWE02].

H [AGI⁺07, BAL⁺01, BPC01, BL00, CPJ00, CS01, DRAS04, GPSP06, HYA02, IN08, IS03, LDMR01, LMK01, LLXS02, LW04a, LYZ⁺08, LMO09, 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, PGRRNG03, PRSMM03, PV07, RFSS06, RWBH09, SOOF05, SEKS09, SLL⁺04a, WDS06, WTKM06, Wei08, Wil01b, WDX⁺02, YTY07, ZY01]. **H-bonded** [LB05, McD08, NL08]. **H-NMR** [AGI⁺07]. **H5N1** [DLRZ09]. **Hairpin** [ZHH09, CJW⁺09, 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-hydroxyformaldoxime** [TT02]. **haloacid** [NYK⁺09]. **haloalkane** [CS03]. **halogen** [BS03, FHF⁺01, GGP09, LZF⁺09]. **halogen-bonded** [LZF⁺09]. **halogenated** [STC⁺08, TZX01b, TZX01a]. **halogens** [TBGRJ04]. **halothane** [TZX01b, TZX01a]. **Hamiltonian** [FGR07, FBLO08, MR02, SAM06, ZWPR⁺04]. **Hamiltonians** [CV09]. **hand** [DFGB09]. **handle** [GCD04, GM04]. **Hansen** [BBG⁺04]. **Haptic** [MR09]. **hard** [TGGP⁺00, ZHMW09]. **hardness** [PRS04, TSSGS07, TSSSG08]. **hardware** [ATMK03]. **harmonic** [CLP⁺05, Ish02, TFN04]. **Harris** [Cul04]. **Hartree** [WMW04, AKN07, Bou00, Cul04, DD00, GAdGM08, MS00, MBWP03, PFJ⁺03, RRS07, WMW03, Wei08, YH07]. **HAsXH** [LS08a]. **having** [WJ00]. **haystack** [BS01]. **HBCC** [BAL⁺01]. **HBOP** [OYH09]. **HBr** [SLL⁺04b]. **HBSITE** [OYH09]. **HCCX** [Mar03]. **HCl** [BL06, WDS06]. **HCO** [JPF⁺00, dRLMS00]. **HCO-L-SER-NH** [JPF⁺00]. **HDMR** [LRWG03, LAR⁺03, LSHR04]. **head** [HSWN01]. **heart** [TKH07]. **heartland** [Sha07]. **heat** [dOMSL01]. **heats** [CS03, JWB05, RCJ02a, WX09, LLA01c]. **heavier** [ZJM⁺07]. **heavy** [BPC01, SL09, WL04, ZX08]. **heavy-metal** [ZX08]. **HeC** [Var09]. **Helical** [CPML08b, Van08, Der00, KF02a, LC09, PCO⁺07b, PCO⁺07a, ZALMG03]. **helicenes** [VKP⁺08]. **helices** [IGNH03]. **Helix** [BRDC02, JS07b, LI07, PP08a, YS00]. **Hellmann** [RLER07]. **hemagglutinin** [DLRZ09]. **heme** [ATBLS04, MBM⁺00, OYH05, RGZM09, RZWS07]. **hemicarcerand** [LMMW04]. **hemoglobin** [MML⁺06, SO07, Sen06]. **Henry** [Sch00, TLOG00]. **hept** [STC⁺08]. **hept-C** [STC⁺08]. **heptafluoropropane** [LDC⁺07]. **heptagon** [STC⁺08]. **heptagon-containing** [STC⁺08]. **heptapeptide** [OM04, YAÇ⁺02]. **herbicide** [XYN⁺06]. **hERG** [MCR08]. **Hess** [YH09]. **Hessian** [KK01a, NKIS02]. **Hessian-free** [KK01a]. **Hessians** [ASWG07, Chu07]. **heteroaromatic** [LLM09]. **heterobimetallic** [RD00]. **heterochiral** [ZOJ⁺06]. **heterocycles** [FSS00, MGMM07b]. **heterofluorenes** [CZFH07]. **heterogeneity** [HS01, ZSC05]. **heterogeneous** [FCK⁺08, ZCS04]. **heterohelicenes** [LC09]. **heterolevel** [EA08]. **heteropentalenes** [CDL06]. **heteropolymers** [SBJ08]. **Heuristic** [DMC05, DLHC06, CAGR08, IZA06]. **Heusler** [GD09, KGD06]. **hexadiene** [PA05]. **hexadiyne** [PWFS01]. **hexagonal** [BK08, LTF⁺07]. **Hexahelicene**

[LC09]. **hexamer** [NK01]. **hexatrienaldehyde** [ZGZX07]. **hexopyranose** [GGK⁺08, LH05]. **hexopyranose-based** [LH05]. **HF** [BRLS12, BRLS08, FKJ⁺01, GKTS04, PMPGP05, WW03]. **HF/6** [FKJ⁺01]. **HF/6-31G*** [FKJ⁺01]. **HF/DFT** [BRLS12, BRLS08]. **HF/MP2** [GKTS04]. **HFCO** [JHPRSM⁺05]. **Hg** [GPSP06, BBI⁺09, WTKM06]. **HH** [CMaGL⁺04]. **HI** [KKJH08]. **Hiberty** [Bic09]. **hidden** [FWH⁺07, HLT⁺05, RP07a]. **hierarchic** [RRS07]. **Hierarchical** [LMH⁺09, CWV⁺05, DJB02, FOK⁺04, LCC09, UIHN09]. **High** [BB08, GAdGM08, LAR⁺03, AZM03, BACJCT01, CCWH02, CN05, DPT03, GL04a, GY08, HGMB04, JJB00, JJB02, KWK⁺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** [CCWH02, KWK⁺00]. **High-precision** [GAdGM08]. **high-quality** [JJB00, JJB02, SSS⁺09]. **high-rank** [RP07c]. **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]. **HLA-DQ8** [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]. **homoconjugation** [MMLC05]. **homogeneous** [FCK⁺08, Pog03]. **homologous** [CC07]. **homology** [KCL06, KVS⁺06, OO08, SGS03, YKK09]. **homopolypeptides** [JS07b]. **homotops** [TDK07]. **Hongxing** [Ano06c]. **HOO** [BL06]. **Hoover** [QNF09]. **hormone** [HMK02]. **host** [CS01, LMMW04, Oos09]. **host-guest** [Oos09]. **Hou** [JW12]. **HOX** [WLLS04]. **HP** [VGDSU08]. **HP-lattice** [VGDSU08]. **HSAB** [PRS04]. **Hua** [JW12]. **Hückel** [Kut07]. **human** [FKU⁺05, HN02, HMK02, LCC09, PDP02, VGDSU08]. **HX** [RB01]. **Hybrid** [BF04, HTN03, WRP⁺06, ZSK07, AAP00, BG00, BBSS06, DMN03, DDBP09, FAR02, FAB⁺00, FMSA06, GRO⁺03, GLD08, HHH00, Han01, ION07, JPCA08, JIK09, KRM⁺02, KN04, LSO04, LWZ09, LS05b, MBM⁺00, MSH⁺06a, PDS01, RDM⁺08, Sza08, THHN01, TFN04, WWL⁺09, XLZ08, ZZL04]. **Hybridized** [SJJ⁺04]. **hybrids** [GXK09, 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, RSP03, UBDPJ04, XLT07].

hydration-parametrized [RSP03]. **hydrazines** [BLN01]. **hydrazone** [Lu09]. **Hydride** [GVATG03, JJH01, LLXS02]. **hydrides** [KS01b, SRB06, dSGCG00]. **hydridotris** [HT05]. **hydrindans** [HKHN08]. **hydrocarbon** [CS01, KFD06, LC06, Wan09, WEE01]. **hydrocarbons** [Bor03, BS03, EB04, FVB08, LS08c, MGMM07a, SDvG01, VS08, WFHP01, WJ00, ZKZ⁺07]. **Hydrodynamic** [BZP09]. **Hydrogen** [AG00, Kle03, RP04, XZ04, ZX04, AD00, AST06, BM07, BUMCMRL00, BL06, CUS00, CUSS03, CPDZH08, CVVB04, CCK01, CDPL09, DR07, EFQD09, GAIMVB01, HdMdS05, HdS06, HRG07, HIA03, HT03, HA04, IO08, JP09, mJZsLyL07, Kle02, LC07, LDC⁺07, LW04a, LDL⁺09, Mck07a, MH08a, NHH05, OO08, PG01, Pac06, PGG06, Pog06, Rao00a, RM07, SPT⁺03, SJW09, TGLL07, WLLS04, WZZ⁺09, Wil01a, WLL⁺03, XLL⁺02, YT04, ZSC05, ZW09, ZH08, ZGZX07, ZX09, vEMK01, vE01, Yos02]. **hydrogen-abstraction** [WLLS04]. **hydrogen-bond** [RM07, SPT⁺03]. **hydrogen-bonded** [CPDZH08, LDL⁺09, MH08a, ZH08, vEMK01, vE01]. **Hydrogen-bonding** [AG00, ZW09, Yos02]. **hydrogenase** [TDH06]. **hydrolases** [OBT09]. **hydrolyses** [DWS⁺09, LYK⁺04]. **Hydrolysis** [WOC⁺03, DLR⁺08, MBL⁺00, RP04, TH02, WJX⁺08]. **hydroperoxy** [BL06]. **hydrophilicity** [DLHC06]. **Hydrophobic** [MBH⁺02, CJDK09, HJCP01, SDL07]. **hydroxide** [CBS⁺03]. **hydroxo** [AZM03]. **hydroxy** [YXZ⁺04]. **hydroxyacetone** [WXX03]. **hydroxyaromatic** [BLO⁺02]. **hydroxyformaldoxime** [TT02]. **hydroxyl** [CUS00]. **hydroxylase** [HLC09]. **hydroxymatairesinol** [SH09]. **hydroxyproline** [BISB02, PRKP05]. **hyper** [Mar03, vGGB00]. **hyperconjugation** [CPDZH08]. **hyperconjugative** [BPC01]. **Hyperpolarizabilities** [MO01, CJK⁺02, LWZ09, Tor02]. **hyperpolarizability** [JPCA08, XWL⁺09]. **hypersurface** [SSBE06]. **hypersurfaces** [PSC⁺01]. **hypochlorous** [JKM08]. **hypothetical** [LD05a]. **hypoxanthine** [KKMMS04]. **hypoxanthine-cytosine** [KKMMS04].

I/O [SSL02]. **ICFF** [KTA03]. **icosahedral** [Eli07, LML⁺00, OSA06]. **IDE** [Gan09]. **IDEA** [DBGV07]. **ideal** [Pan07, STSF02]. **ideal-gas** [STSF02]. **identical** [CSD05]. **Identification** [CP09, FWH⁺07, KS05b, PXP01, SLC⁺09]. **identify** [LHJ⁺06, ZS04]. **Identifying** [CCCJ09, DB02, CLS⁺09, HLT⁺05]. **identity** [DSR⁺07, Nee03, RC04]. **idiosyncratic** [CMCB08]. **II** [ACM⁺06, DPT03, DF04, FNP⁺06, FKŠ⁺09, GPK05, LPP06, NK06, Sha02, TGGP⁺00, WM01, BHW00, BA04b, Ber03, Car02, CSB08, EBD⁺01, EKB02b, GGB07b, HZ06b, Ish03, JJB02, Kle03, LLA01a, LFZS04, LCDA03, LMIF06, MB00, OBBS05, PMB04, PV03, Rud05b, TJM⁺03, TCR⁺02, WHP02, WNH03, WFR08, vEMK01]. **III** [BB08, DF04, FRS05, KPR04, VHRR07a, YIN03, CCB04, CG05, KEB04, LLA01b, LCGA03, ZFL⁺05, vE01]. **Illustration** [KS02a]. **image** [IC08, XWC09]. **IMiCMO** [MS01]. **imidazole** [JKM08, PGG06]. **imidazoline** [XKG⁺05]. **imide** [CXZ⁺09]. **imine**

[Bor03, GTC06]. **imipenem** [SDM02]. **immune** [WCS09]. **immunoglobulin** [Kr603]. **IMOMO** [VM00]. **IMPACT** [BBC+05]. **Implementation** [AKN07, CKW09, DRMD03, KBT03, LI07, PZS04, RNG03, SVT09, YTH+07, BMRDB01, BLMS08, DFWH05, 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** [Ano06a, JS07b, KS05c, CBH+03, NHH05, ST06]. **implicit** [BBHD04, BLL+06, GL04a, JS07a, JZD+09, KTA03, Kr603, Lab08, LSO04, MCM04, PZS04, PPYS08, SBLK01, SL06, WL09a, ZGFL01]. **Importance** [CGBF05, ENM+04, ZM06, HLC09, JW06, OCB02, PMPGP05, PMM05, TS05]. **important** [CSU05, EDAJ04, Tor02]. **improper** [TNS00]. **improve** [FSM09, XLT07]. **Improved** [CN03, CLA+00, Gri03, HQ02, KK08a, KK08b, LK04, RCJ02a, SKSH07, TGD05, Wil01a, Wil01b, CMBC08, DSR+07, KDSV02, MP03b, Maz08, MFR07, PABK03, PRS04, SDvG01, STSF02, SHK+05, VZM+08, LK03, RCJ02b]. **Improvement** [SM08b, UKN04, Nee03]. **improves** [CLWL09, RK05]. **Improving** [BUMCMRL00, Bie04b, GF08, LJ04, LKW04, GRO+03, GP06, SMG09]. **in-core** [FR06]. **inactivation** [PFR04a]. **incidence** [YWHZ03]. **InCI** [ZL05]. **Including** [IC08, AKN07, DP03, DP04, Gri04, Ish03, LB08, SL09, Wil01a]. **Inclusion** [HK08a, HK08b, PWHF+03, PWHF+04]. **incomplete** [FWH+07, Ish04]. **incompressible** [ZHMW09]. **incorporate** [KTA03]. **Incorporating** [CLS+09, DMJV05, HLT+05, SLC+09, HS01, LL07, RD06]. **incorporation** [SM06]. **Increasing** [ZWZ09, BT00, LJS05, YAÇ+02]. **independent** [FVB08, OTL08, Van02a]. **index** [COS01, JLHF03, MBH+02, PVdJB00, Pog03, YWHZ03, YWH04, YYW07]. **indexing** [HWDB03]. **indicators** [BWW+08, HIM07]. **indices** [BLT03, CGMPT+08, FZL07, FMPS08, FVB08, FS04, GDPCPU07, MGMM07a, MGMM07b, May07, Rao00a, SPGS08, TSMNG01, TSSSG08, WMW03, WW03, WMW04]. **indium** [ZL05]. **individual** [ZM06]. **INDO** [PBZ00, TY03]. **INDO/SCI** [TY03]. **indole** [LL01]. **induced** [CGB03, CMCB08, EDW07, HIM07, HHP04, KIFK07, LGB+09, LBG08, MLA00, PSF+08, RSN+02, ST01, ZALMG03]. **Induction** [HK08c, HK08d, ZOJ+06]. **Inductive** [BE07]. **inelastic** [BACJCT01]. **inexact** [Har04]. **inexpensive** [KFZ03]. **infinite** [DA01]. **Influence** [GSB09, JS07a, JT08, LZA02, BGC+09, SBH02, SLRC01, DB06, EL09]. **Information** [Ham07, GCB03, HTKG08, HP05, NL08]. **information-bearing** [NL08]. **infrared** [CVR08, Kle03, LDL+09, MGLDS00, TDH06, Zer08]. **Inherent** [BYQS03]. **inhibition** [PFR04b, WC08]. **Inhibitor** [VVS07, BMTFR08, CWV+05, FPG+06, MBC08, SVV+08]. **inhibitors** [AJNG01, AGO+02, APG05, AVS09, LLL+08, LZ05b, PB06, RGP+07, VB09, VVS07, WZY04, WHF08, ZWB09]. **inhibitory** [DD08]. **inhomogeneous** [MZL08]. **initial** [MM03, MABM09, Qua07, UNM+01]. **initialization**

[FKFG08]. **initiated** [RAGLL09b]. **initiation** [GGGLL05]. **initio** [AJ03, Ama02a, Ama02b, Ano06b, ASY01, BG03, BG00, BL08, BSB05, BS01, BL06, BLO⁺⁰², BSJ01, BZL05, CPJ00, CPM03, CUS00, CU01, CUSS03, CLC09, CYM02, CJW⁺⁰⁹, CHRL09, DGD⁺⁰⁵, DWS⁺⁰⁹, DPM09, DB06, Dra00, EM03b, FG02, FAR02, FO08, FNP⁺⁰⁶, FKU⁺⁰⁵, FKM⁺⁰⁶, FKM⁺⁰⁷, FKŠ⁺⁰⁹, GKRG08, GD06, GBB07, GGLR00, GKTS04, GPK05, GBBH09, Haf08, HSF08, HYA02, HELM09, HSMT04, HMSM06, HFHL06, HS07a, HTSR04, HRR05, HSWW00, HJCP01, ITS05, ITS06, JCA⁺⁰², JFG04, JČHS07, KSB⁺⁰², KP05, KFNH08, KKG⁺⁰⁹, Kle02, KF02a, KIFK07, KWK⁺⁰⁰, KPR04, Kri08, Kri09b, LMK01, LYK⁺⁰⁴, LDC⁺⁰⁷, LMCD09, LMB08, LZJ03, LWLS07, LKT04, LF02, LXSf08, LLL07, LZF⁺⁰⁹, LMO09, Mar03, Mas01a, Mas01b, MDA08, MGLDS00, MLL^{+08b}, MM02, MS00, MA09, MG00, MLCD01, MW00]. **initio** [MS01, Mor02, ML00, Mui05, NYK⁺⁰⁹, OO04, OON01, OS08, ON07, OO08, PP08a, PGNG03, PGRRNG03, PHRR08, RSSKB03, RSE07, RRCA08, ROG00, RGG08, SS00, SG07a, SAS05, ŠBL05, Sha02, SLL^{+04a}, SSS⁺⁰⁹, SRE08, SMK00, SMZW05, SK05, SSBE06, TAS07, TYN05, TZX01b, TZX01a, TGGP⁺⁰⁰, TFZRG01, UCT⁺⁰³, UM03, UTM⁺⁰², VSK⁺⁰⁴, VS02, VIP⁺⁰⁶, WMGK07, WLLS04, WLL07a, WS05b, WOC⁺⁰³, WDX⁺⁰², WXX03, WCL05, XLL⁺⁰², YXC⁺⁰⁷, ZSE08, ZZL04, ZZZ⁺⁰⁶, ZWZ09, ZGXX06, ZX08, ZWTP⁺⁰⁸, ZL09b, vDSSvA04, vEMK01, vE01, CSV⁺⁰⁷, MDI04, SH07, TBG00]. **inner** [Pog03]. **inner-core** [Pog03]. **inorganic** [CMA⁺⁰⁸, SYY⁺⁰³]. **inserted** [BL08]. **Insertion** [ZZvRSC08, 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, BRS00, BRS01, CC09, CJDK09, CF04, DBS08, GWM08, JP09, KJVW08, Lab08, MBWP03, SVT09, UKN04, Vya01, Yas08, PVdJB00]. **integral-driven** [SVT09]. **integrals** [ABF⁺⁰³, FL08, FMAMVK06, FR06, GGA00, Ish03, Lai07, RLER04a]. **integrands** [GC03]. **integrate** [MP03a]. **Integrated** [BBC⁺⁰⁵, HT03, LOL⁺⁰⁸, MS01, VKCK09, VM00]. **integration** [BK00, Blo04, CLF⁺⁰⁹, ESP04, HW03, JCA⁺⁰², KBA⁺⁰⁴, LRWG03, Pom04, RP07b, SY09]. **integrations** [PFB05]. **integrator** [CF06, KM00, QNF09]. **intensities** [WKYU01]. **Intensity** [Tor02]. **Intensity-carrying** [Tor02]. **Inter** [HRBKB03, MAF⁺⁰⁷, RP02, SWV⁺⁰⁵]. **Inter-** [HRBKB03, RP02, SWV⁺⁰⁵]. **inter-phycoyanin** [MAF⁺⁰⁷]. **interacting** [RGG08, YCXY03]. **Interaction** [BE09, GBBH09, LSAS01, MHS05, ROG00, AKN07, ABĀ04, AZM03, BRLS08, BRLS12, CLC09, CF04, CFC⁺⁰⁸, CPML08a, DLD⁺⁰², DMZT08, FK07a, FL07, GDV03, GWM⁺⁰⁰, GS04, GKTS04, HZ06a, IDMC09, Ish03, KN04, KBT03, KS05c, LDMR01, LWX07, LPB03, MLL06, MN02, Mas04, NTH09, Oos09, PPXP01, PMPGP05, PRSMM02, PRSMV08, RRCA08, SKGS00, SSL02, SYC03, SWZS04, SLRC01, TKH03, UTM⁺⁰², VC04, WS05b, ZCZ03, ZWP08, EB04, JČHS07, LFZS04].

Interactions [CPML08b, FKŠ⁺09, Van08, ALC08, AG00, ASDP⁺06, ATMK03, Ano05b, AS00, BPC01, BM07, BUMCMRL00, BSJ01, CMàGL⁺04, CEP07, DDBP09, EFQD09, FÁ01a, 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, RZWS07, SOOF05, San01, Sha05, SSS⁺09, SWV⁺05, SG01, SL06, SDL07, SMV⁺09, UTT⁺04, VW03, WRP⁺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, HHH00, HZX04, JKII08, KKG⁺09, LLL02, LPB03, PHJ⁺08, SWM04, TdMSD⁺08, ZCS04, DBGV07]. **interfaced** [FKL⁺06]. **interferences** [BSH07, ZZTS09]. **interfacial** [CW02, MWL⁺08, PHJ⁺08]. **Interfacing** [WHG⁺07]. **interior** [SYC08]. **interlayer** [ALC08]. **interlayers** [DJT08]. **intermediates** [BLO⁺02, BMTFR08, IGNH03, MMY07, OBT09, WSM⁺09]. **Intermolecular** [PSC⁺01, AS00, CMàGL⁺04, CLC09, FÁ01a, FKM⁺06, FKM⁺07, GGP09, GS04, IGL07, KS05c, LZJ03, Mas04, PMPGP05, RRCA08, SPDS01, SJW09, UTM⁺02, UTT⁺04, Wil01a, Wil01b, ZDS⁺05]. **Internal** [EA06, BHH⁺09, CFD03, CFD04, COMR⁺04, DHF⁺05, Din00, HFSD03, KSU03, KTA03, LPK07, MGLL03, NKIS02, SWR06, TNS00, WR07, WFR08]. **internal-rotation** [DHF⁺05]. **interparticle** [PK05]. **Interplay** [EFQD09, SP05]. **interpolated** [YK08]. **interpolation** [BB05, IS03]. **interpretation** [CPJ00, HLS07, VM07]. **intersection** [SSHT03]. **intersections** [IK00]. **interval** [LS05a]. **interwall** [ZZvRSC08]. **Intra** [FÁ01a, FKM⁺06, FKM⁺07, MAF⁺07]. **Intra-** [FÁ01a, FKM⁺06, FKM⁺07]. **intra-phycoyanin** [MAF⁺07]. **Intramolecular** [GKTS04, HA04, PG01, TFZRG01, AGK03, BA03, BA04a, FDSA00, HRBKB03, HK08d, Li01, NHH05, 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, Nil09]. **inversion** [KSTC01, RC04, ZSE08]. **investigate** [DWNB01]. **investigated** [HN02, Kle03, YH09]. **Investigation** [LZZC09, YTH01, AST06, BL00, CW02, CHA⁺07, CG08, FG03, GS04, Hir08, JJH01, KYFW07, LH02, LXSF08, NSB08, PV07, QZZZ03, QZL⁺04, RM07, RC04, RY09, SL04, TGGP⁺00, TFZRG01, UCT⁺03, WL09b, WLZ⁺07, ZXY08, ZKZ⁺07, ZHMW09, ZGZX07, GBJ03, JBGK08]. **Investigations** [JP09, WG02]. **involvement** [BLO⁺02]. **involving** [LL01, MM05, ZGZX07]. **iodides** [CM09]. **iodine** [GWM⁺00]. **iodobenzoylphosphonate** [GWM⁺00]. **Ion** [DAK08, BM08, Dra00, EL07, FHRR07, FL07, GWM08, Gor01, IvSV06, KPR04, Kri08, Kri09b, MSBS01, PPYS08, PHRR08, RC04, VHRR07a, VHRR07b, ZZW09, dOMSL01]. **ion-pair** [RC04]. **ionic** [Ang09,

BM08, BSG07, BGJ01a, CFC⁺08, DMJV05, GGT08, HTN03, LR03b, Loe03].
ionizable [OS06]. **ionization** [GSB09, KFD06, RTG00, SVT09].
ionospheric [LSHR04]. **ions**
 [CXZ⁺09, DMJV05, EL06, FG03, HTSR04, HLB09, JRJ01, KT08, KZRO03,
 LSWB00, LMIF06, MHS05, RMP01, SL09, ZSC05, ZZZ⁺06]. **IPR** [GZ07].
IR [NRKH02, ZWTP⁺08]. **iron** [DPT03, GK09, HLLN06, LWH06,
 MSH⁺06b, OYH05, RJLR06, SW06, TGLL07, TDH06, CN05, LPP06].
iron-containing [MSH⁺06b]. **irregular** [ZBS03]. **irrelevance** [VVBV02].
ISBN [Bic09, Lip00, Sta00]. **ISBN-10** [Bic09]. **Iso** [GWL07, Rap06].
iso-energy [Rap06]. **Iso-guanine** [GWL07]. **isobaric** [SM03, Ste04].
isoconversional [CC09, Vya01]. **isocyanates** [OY01]. **isocyanide** [HT05].
isocyanurates [OY01]. **isoelectronic** [Che01]. **isolated** [RZWS07]. **isomer**
 [HLLN06]. **isomerase** [AGK03, GVATG03, RGP⁺07]. **isomeric**
 [GCCVB00, XFF06]. **isomerism** [ACM⁺06]. **isomerization**
 [Lu09, ML00, Qua07]. **isomerization/decomposition** [ML00]. **Isomers**
 [Ber03, CCB04, GB02, CDL06, CTFC08, HYA02, KYFW07, KZY09, LS08a,
 LMO09, Sau04, ZZZ⁺06, ZZvRSC08]. **isomorphic** [CRGN07]. **isoprene**
 [Dib05]. **isoprene-OH-O** [Dib05]. **isothermal** [SM03, Ste04].
isothermal-isobaric [SM03]. **isothianaphthene** [CFD04]. **isotope**
 [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, FSFK05, Pul05, 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**
 [BRS00, BRS01, DDVD09, TSSGS07, TSSSG08]. **kernel-based** [DDVD09].
ketene [MGG06]. **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].
kinase-channel-phosphatase [FCP⁺05]. **kinase-specific** [HLT⁺05].
kinases [SWM04]. **kind** [LX07]. **kinematic** [CSJD04]. **kinematics**
 [CCC03, LFKL00, MLL08a]. **kinematics-based** [LFKL00]. **Kinetic**
 [mJZsLyL07, Bie04b, BZL05, GWM08, Jac09, Kri09a, WDX⁺02]. **Kinetics**
 [CUS00, ST04, Gog08, HLSH05, 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, Bou00, SH02]. **Kollman** [JVVK09]. **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-peptides** [OYK⁺09]. **L-phenylalaninamide** [HJCP01]. **L-valinamide** [HJCP01]. **La/SSB** [KVS⁺06]. **label** [VCM01]. **labeling** [SN00]. **lactamase** [AGO⁺02, APG05, SDM02]. **lactamases** [ESM06, MK02]. **LADH** [DMC05]. **LaN** [VP08]. **Lanczos** [MO01]. **Landau** [GHH07]. **landscape** [IGNH03, PAT⁺09, SPL⁺02]. **landscapes** [OKH⁺02, SSB07]. **Langmuir** [BRS00]. **lanthanide** [AB00, FRS05, RMP01, SNM⁺06, VMA03]. **lanthanides** [RD06]. **Lanthanum** [AB00]. **Large** [WCF04, ARL01, AB08, AS00, BG03, BP01, BdPRMAI00, BME05, CJK⁺02, CDD⁺02, CG06, DMN03, DJB02, Ell07, FZL07, HB09, HMSM06, IME02, IS07, JO02, JW00, KS05b, KKG⁺09, KK01a, KH06, LMJ02, MKGA06, MH09, MHW04, MH08b, MPF00, ME06, NRKH02, PFJ⁺03, RRS07, SYC08, SSL02, TYO⁺02, VSK⁺04, WWL⁺09, YCS07, vGGB00, WS07]. **large-amplitude** [KS05b]. **Large-scale** [WCF04, DMN03, JO02, KK01a, MH09, MHW04, MPF00, ME06, RRS07, SSL02, TYO⁺02]. **larger** [VKP⁺08]. **lariat** [ZWY⁺09]. **laser** [Sha02, KZW⁺05]. **latency** [KVF⁺07]. **latter** [LPK07]. **Lattice** [OGH05, SG01, HP01, KWK⁺01, KWK⁺02, KF02b, LJKL08, MH08a, SCC04, SYC08, TK08, VGDSU08, YCS07, vE01]. **law** [Sch00]. **LCAO** [EBL⁺08, EL09]. **LDA** [RLDI09]. **lead** [RS07a, RS07b]. **leads** [PPXP01]. **learning** [YCW⁺09]. **least** [CSD05, Gol09, LLZL09]. **least-square** [LLZL09]. **LEDO** [GKH05]. **legacy** [Sha07]. **Lei** [Ano06c]. **length** [CRC⁺08, DR09, JPCA08]. **length-frequency** [DR09]. **lengths** [PSC⁺01]. **Lennard** [CYM02, FSFK05, Pul05, SCC04, SYC08, YCS07]. **Lennard-Jones** [CYM02, FSFK05, Pul05, SCC04, SYC08, YCS07]. **lesion** [Pin01, SHD⁺08]. **lesioned** [Pin01, Pin03]. **Letter** [BFS07]. **Letters** [JW12, WM12, vLBBR12]. **level** [BUMCMRL00, BLT03, BL00, DPM09, JMD⁺02, mJIZsLyL07, KK08c, PFJ⁺03, RC04, TBG00, TST⁺08, UTM⁺02, WyLG⁺09, WS05b, WLL⁺03, ZZL04, ZWL⁺05]. **levels** [BACJCT01, Cul04, DJB02, PFJ⁺03, WW03]. **Lewis** [BHTCG07, GR07, Sha07, Sim07]. **LF** [PWHF⁺03, PWHF⁺04]. **Li** [CRC⁺08, GBDP05, JW12, HDO⁺02, LWK08, LWW⁺06, LAT05, WWT08]. **libraries** [AL01, KV00, LZ05b, ZMZ09]. **library** [CRH⁺07, FAB⁺00, KSM05, OTL08, SH07]. **LiF** [EL09, UM03]. **lifetime** [CHA⁺07]. **Ligand** [MKT04, AM06b, BSP06b, BGC⁺09, BS08, BMTSC01, CGB⁺09, CLH⁺07, CN05, DFWH05, FO08, GZM09, HZ06a, HZ06b, HW09, JZD⁺09, KS08, LXW⁺09, Mue01, NR04, NMAT01, OFIK09, PWHF⁺03, PWHF⁺04, RK05, Ruv07, SOOF05, STSF02, TFN04, TJE03, VGGMM05,

XZZ04, YK00, Yan04, ZGFL01, ZWS⁺02, BDW00, HLC09]. **ligand-charge**
 [BSP06b]. **ligand-protein** [VGGMM05]. **ligands**
 [BS05, CKMC04, FO08, FKU⁺05, GTC06, GM01, GGLR00, JFG04, RGG08,
 SWM04, TP01a, TGGP⁺00, WS02b]. **ligation** [KT08]. **light** [Kr03, LFR07].
light-emitting [LFR07]. **lignin** [PS09b]. **LiH** [McD03]. **like**
 [BCIB05, DHW⁺00, DB02, FZL⁺06, JD09, Kut07, LAEL01, PRKP05, WL09b].
limit [MV06, MLL⁺08b, PSC⁺01, SAS05, Var09]. **limitations**
 [BYQS03, LFE06, PRDS08, MFB04]. **limited** [Ano05b, Sha05]. **Limits**
 [OV03]. **line** [RHL09]. **Linear** [Con02, DLWV07, KDG⁺09, LMJ02, OS06,
 OFIK09, SKDO08, vdVGDM00, AT02, AB04, 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** [Sta00]. **lipophilicity**
 [DMC05, DLHC06, DLHC06]. **lipoxygenase** [TGLL07]. **lipoxygenase-1**
 [TGLL07]. **LiPt** [LWK08]. **liquid** [BM08, CC07, EGSG00, GDV03, GJK00,
 HPL03, MN02, MM07, NL07, PHJ⁺08, PB04, POJ01, YGLvG06].
liquid-state [POJ01]. **liquids** [CF04]. **list** [PABK03]. **lists** [KUB07].
lithium [HXD08, LWLS07, RC04, SLRC01, YSA⁺03]. **liver** [CMCB08].
LMO [BY06]. **Local** [Din00, LYS08, AGSFAL05, CPML08a, ION07, IS03,
 JHPRSM⁺05, KMA⁺07, LMJ02, MA09, PMC⁺08, RUPH06, SL09, SEKS09,
 SB08, TT05, TSSSG08, VKCK09]. **localizability** [BK08, BWW⁺08].
Localization [Che01, ALTB06, FS02, FSS00, GBJ03, PP08b, 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**
 [ABBC01a, ABBC01b, Bof01, GMA04, MP03b, Qua01]. **locating** [WSM⁺09].
Log [Tot04]. **London** [Lab08]. **Long** [RP07c, CCSJ00, CPC⁺00, CEP07,
 CSRST04, Gri06, KSS08, LYS08, MN02, MBC08, RLP08, San01, VVBV02].
long-duration [CCSJ00]. **long-range**
 [CEP07, Gri06, KSS08, MN02, RLP08, San01]. **long-time** [CPC⁺00]. **lookup**
 [Nil09]. **loop** [CSJD04, KK01a, Mak08, OFB08, PRT⁺07, PRT⁺08, TLKT00].
loops [CSRST04]. **LoProp** [SKK⁺07]. **Low** [DPT03, MG06, AG00, BS05,
 GS03, KUB07, KK01a, KK01b, LAR⁺03, LBG08, LB08, PFJ⁺03, PRSMV08,
 Rao00b, Sha02, WS02b, ZL05, ZL07, ZL09b, dSVA⁺09, BS08]. **Low-**
 [DPT03]. **low-energy** [Rao00b]. **low-level** [PFJ⁺03]. **low-lying**
 [LB08, ZL05, ZL07, ZL09b, dSVA⁺09]. **low-mode** [KK01a]. **low-resolution**
 [BS05, WS02b, BS08]. **lowest** [FDSA00, OSA06, XZ04, ZX04]. **lowest-lying**
 [FDSA00]. **lp** [LAR⁺03]. **lp-RS-HDMR** [LAR⁺03]. **LR** [ZWB09, NSO⁺07].
LR-MMPBSA [ZWB09]. **LSCF** [FAR02]. **Lu** [SNM⁺06]. **lumiflavin**
 [CNN07]. **LUMMOX** [MS04]. **lutetium** [AB00]. **lyase** [PMM05, ČJPZS08].
lying [FDSA00, LB08, PRSMV08, ZL05, ZL07, ZL09b, dSVA⁺09]. **LYP**

[PDS01]. **Lysine** [DJT08]. **lysozyme** [HN02].

M [Bof01, GPSP06, JJK+00, LYZ+08, OS08, Qua01, WWC+05, JJK+00, LMGR06, OS08]. **machine** [CLS+09, HL08, LJZ+07, YCW+09]. **machines** [CLXC02, QLHL09, YMT04]. **macro** [Wou00]. **macrocycle** [RRZA08]. **macrocycles** [FLOD07]. **Macrocyclic** [SCG04, KB02]. **macromolecular** [Ara04, Con02, EA06, FM00, JO02, KS01a, KHY00, RP07d, ZBS03]. **macromolecule** [BVW04, HMWC03, YH06]. **macromolecules** [BTLP03, BR03, BH03, EM03b, HHS+05, Mac04, PPXP01]. **macropolyhedral** [ZZZ+06]. **Macrotricyclic** [CW02]. **Magic** [KZW+05, HXD08, KKJH08]. **magnesium** [ZZW09]. **magnetic** [BACJCT01, CDL06, CDPL09, DXW08, HWFN01, HIM07, KCL00, KGD06, MV06, MDI04, PJPJdPRMI07, QTdG+08, RLDI09, TDK07, WZXY07, ZPL07, ZXY08]. **magnetism** [Hua09b]. **magnetizabilities** [YH07, YH09]. **magnetizability** [CDL06]. **magnets** [FKRE08, SM08a]. **MAGPACK** [BACJCT01]. **main** [Din00, JGH00, LW07]. **main-chain** [Din00]. **maingroup** [SRB06]. **maingroup-element** [SRB06]. **Maintaining** [LFBSK07]. **maleimide** [RP09]. **malonyl** [LLL+08]. **malonyl-CoA** [LLL+08]. **maltose** [MW00]. **maltotriose** [SWBM08]. **Manager** [FCK+08]. **manganese** [AZM03, CWY09, GK09, LMIF06, LS05b, RJLR06]. **Many** [Loe03, BM08, TKH07, YCXY03, LR03b]. **Many-body** [Loe03, TKH07, LR03b]. **many-electron** [YCXY03]. **map** [MLL08a, SKGS00, HLTLP09]. **mapping** [FKZ09, RLA01]. **maps** [PRT+07, PRT+08, TTB01b, WD04]. **Marchi** [Ano06b]. **Marcus** [BLN01]. **Markov** [BHG03, CPUGD09, CMGDAC+07, DLW06, FWH+07, HLT+05, SK09]. **Markovian** [YCXY03]. **mass** [GM04, Gor01, KZW+05, LHJ+06, ZWZ09]. **masses** [CN03]. **Massimo** [Ano06b]. **Massive** [TP01a, RLA01]. **massively** [DGHR02]. **master** [FR06, FS00b]. **master-slave** [FR06]. **matching** [SMM+08, VSW+03]. **Material** [JW12, SLHW09]. **materials** [BCF+09, Haf08, LLXS02, LMRVFH+09, Tie09, XK08, YPNE09]. **mathematical** [DDVD09]. **Matrices** [LSAS01, AT02, BdPRMAI00, CZA03]. **matrix** [CGSdST06, Ell07, GHH07, IS07, JCA+02, Li01, NKIS02, Nee03, RS05, RRS07, RRS09, SK09, SSB+03, TYO+02, UIHN09, YWHZ03, vDSSvA04, vW06]. **Matteo** [Ano06b]. **matter** [ASDP+06]. **maxima** [MSH+06a]. **Maximal** [GCDL+05]. **maximization** [BWI+02]. **maximizing** [AM07]. **Maximum** [MWE02, SCS07, HXD08]. **MBO** [CPC+00]. **MC** [HMD06, MLG04]. **MCCE2** [SMG09]. **MCDP** [LAEL01]. **McLafferty** [NSB08]. **MCM** [NCO+05]. **MCPRO** [JTR05]. **MCSCF** [IR03]. **MD** [KIM+09, MDA08, ALB09, BMRF01, CADW03, HRR05, Höf05, PHRR08, WRBV03]. **MD-based** [BMRF01]. **MD-GRAPE-2** [Höf05]. **MDGRAPE** [KAK+09, NYTH09]. **MDGRAPE-3** [KAK+09, NYTH09]. **MDSimAid** [CHMI05]. **mean**

[GMA04, HFSD03, LHI09, MMLC05, NMAT01, RNG03, YCXY03].
meanfield [KRM⁺02]. **meaningful** [AE06, Bud07]. **means**
 [Bac05, Bie04b, BLF02, Kar06, KBL08, SMA0V00, WKYU01, dOMSL01].
measure [XSHC06, ZHH09, PDC⁺08]. **measurement** [YZ04].
measurements [KBLP09]. **measures**
 [BDW00, DW08, Ham07, Leh06, PYEA03, PCA⁺08, PDC⁺08]. **mechanical**
 [AVB00, BISB02, CLP09, CGBF05, CCK01, COL⁺06, DWC⁺03, ECA06,
 ESM06, EBD⁺01, FHRR07, FÁ01a, FAB⁺00, FKU⁺05, GAIMVB01,
 GGLR00, JJH01, KKS04, MP03a, MBL⁺00, Sau04, TCR⁺02, VHRR07a,
 VHRR07b, XZZ04, XLZ08, YPNE09, ZCZ03, ZAT07].
mechanical/molecular
 [CGBF05, FÁ01a, TCR⁺02, VHRR07a, VHRR07b, XLZ08, ZAT07].
mechanics [AS06, AS09, AD00, AM06b, AGO⁺02, APG05, BDW00,
 CLFA07, CR02, CSU05, DPT03, DFWH05, DWC⁺03, EC06, FEVM01,
 GCD⁺08, GS04, GKTS04, GPK05, HWTL03, JČHS07, KLB03, KZRO03,
 LL00, LLA01a, LLA01b, LLA01c, LLA01d, LLA03, LSWB00, MLA00,
 MFB04, MPF00, OSHS03, PRKP05, PS09b, PWHF⁺03, PWHF⁺04, RMP01,
 RSE07, RP02, ROG00, RM00, RGP⁺07, SS00, SHD⁺08, TGGP⁺00,
 TFZRG01, TT05, VSW⁺03, XOW⁺00, YSA⁺03, ZSK07]. **mechanics-based**
 [BDW00, RSE07]. **mechanics/molecular** [MPF00]. **Mechanism**
 [CJK⁺02, LWY⁺09, PFR04a, Rao00a, AM07, AGK03, BTP09, BLO⁺02,
 BS03, CGB⁺09, CBS⁺03, DBS07, HP04, HLB09, mJlZsLyL07, JDWS06,
 JJH01, LMGO⁺09, LPP06, LL01, LDT⁺02a, LDT⁺02b, LYZ⁺08, LFS⁺07,
 MCK05, Mui05, PGNG03, PFR04b, PS03, PMM06, wQZsLyZ02, QZZZ03,
 RJLR06, SMKM00, gThDjL⁺01, WDWS06, WCW08, WCHW09, WXX03,
 WJX⁺08, YQQH09, ZLLS04b, ZLLS04a, ZLLS05, ZLLS06b, ZKZ⁺07,
 ZGZX07, GVATG03]. **mechanism-based** [PFR04b]. **mechanisms**
 [AGI⁺00, AGI⁺07, BS06, CCCJ09, CG05, ILKR09, KZY09, KKJH08,
 LLKC06, MK02, NSB08, RC04, Sie01, TMBM02]. **Mechanistic**
 [BMTFR08, SGS03, TT02, Ano06a, ST06, WDS06, XDS06a, ZLLS06a].
media [HLLN06, MM02, SMKM00]. **mediated** [HIA03]. **medium**
 [FZL⁺06, HXLS09, LF04, LFZS04, SHH07, ZFL⁺05]. **medium-resolution**
 [HXLS09]. **medium-sized** [SHH07]. **melatonin** [CKT⁺08]. **mellitus**
 [PS09a]. **Melting** [LML⁺00, KT02]. **membered** [FJ08, ZW09]. **membrane**
 [ALB09, CJDK09, DAK08, FCP⁺04a, GAS04, ILKR09, JM07b, LPB03,
 MHJS06]. **membranes** [Ike04, SSM08, WC09]. **memoriam** [Ano00].
memories [WHRG08]. **memory** [TYO⁺02]. **mercaptocarboxamides**
 [TFZRG01]. **mercaptocarboxylate** [APG05]. **mercaptopyridine**
 [YXZ⁺04]. **mercury** [FNP⁺06]. **Merging** [PJPJdPRMI07]. **Merz**
 [JVVK09]. **Merz-Kollman-Singh** [JVVK09]. **mesh**
 [BYQS03, KM00, KSY⁺00]. **mesoscale** [RPMP03, ZBS03]. **Mesoscopic**
 [YPNE09]. **Met-enkephalin** [ZCL09]. **meta**
 [DDBP09, ION07, ZTP⁺08, Gan09]. **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, Hol05, HSWW00, IC08, JHMB⁺09, JHMB⁺11, JKL08, KT08, KRM⁺02, KEM08, LW07, LML⁺00, LWK08, LMGR06, LS02, LWZ09, MSBS01, NR04, PYCD03, PLC08, RRFC⁺03, SL09, SZT08, ST06, TAS07, VHRR07b, WB07, WWT08, Wu06, YTH01, ZSC05, ZWY⁺09, ZX08]. **metal-catalyzed** [HSWW00]. **metal-free** [CM09]. **metal-organic** [TAS07]. **metal-porphyrins** [LS02]. **metal-rich** [LWK08]. **metallic** [ALC08, KWK⁺01, KWK⁺02, SK08, WLX⁺05, WL09b, dVB01]. **metallo** [AGO⁺02, APG05]. **metallo-** [AGO⁺02, APG05]. **metalloenzyme** [BSDM04]. **metalloenzymes** [Sie01]. **metallofullerene** [CTFC08, KJP⁺07]. **metallofullerenes** [KSN01]. **metalloproteins** [CR09b, SN06]. **metals** [BP03, BGJ01b, CM09, LD05a, LK03, LK04, WLX⁺05]. **metathesis** [PHKG07]. **Methane** [RRS06, CLC09, EL06, EL07, EM03a, LLN06, HYR06, IME02, PV07, TMBM02, YQQH09]. **methanediamines** [CPJ01]. **methanol** [CCK01, YGLvG06, ZH08, ZWP08]. **methionine** [BTP09]. **Method** [KFB05, MO01, YGZZ05, AKN07, ABÅ04, AE06, Ami00, ATMK03, AB09, Ano05b, Ara04, BL09, BWP07, BP01, BVW04, BCNs07, Bie04b, BH03, BF04, BM00, BGC⁺09, BHG03, BHH⁺09, CC09, CCL06, CSJ01, CG03, yCkHmY08, CRG01, CPC⁺00, CAG07, CA04, DPT03, DRMD03, DPRR05, DMLI05, DDVD09, ECM⁺03, FOK⁺04, FKL⁺06, FII⁺07, FÁ01a, FAR02, FS00b, FSFK05, FRLN09, FKU⁺05, GMA04, GS09, GY06, GB04, HDBD04, Har04, HFS⁺07, HHS⁺05, HNWF07, HNWF12, HQ02, HDF⁺07, HSWW00, IIK09, IR03, IK00, JO02, JVVK09, KKY01, KDG⁺09, Kar01, KTA03, KN04, KM00, KLS02, KKC05, KSY⁺00, KK08c, Kol04, KIM⁺09, KBB09, KLM⁺09, KC01b, LSO04, LRWG03, LR06, LWX07, LZZC09, LXW⁺09, LCSZ09, LZ05b, MLL06, MKGA06, MKT04, MBM⁺00, MCF05, MSH⁺06a, MH08b, MG00, MS01, MY08b]. **method** [MPF00, MRS⁺07, NKIS02, NA06, NGTB03, NG04, Nye07, OM04, PHJ⁺08, PABK03, PMC⁺08, PZS04, Qua07, RNG03, Rao00b, RSE07, RLR⁺04, RK05, SK09, SMAv00, Sch04, SCC04, SYC08, Sha05, SF05, SG07b, SWZS04, SVT09, THHN01, TFN04, TVL⁺03, TY03, TKN⁺08, VK06, VZM⁺08, VM00, Vya01, WS05a, WCC08, WW03, WLZ⁺07, WL00, WBSR03, WM04, WX09, XL02, Yan04, YZ06, YCS07, YAÇ⁺02, YH06, YH07, YH09, YXL⁺09, ZWS⁺02, ZL09a, vdVGDM00, JBB00, KTM02, SRCD03]. **method-based** [KIM⁺09]. **methodological** [FDSA00, MFR07]. **Methodology** [KS02a, SPL⁺02]. **Methods** [LSAS01, SB01, AJ03, AGMPRG⁺08, BB05, BL05, CMàGL⁺04, CG05, DLD⁺02, DB07, DMN03, DBM03, DDBP09, FOL⁺04, FO08, GHLK⁺02, GHH07, GY08, GD09, GPN01, GGLR00, GHBB04, HTKG08, IB04, JFG04, KK08b, KBL08, Kle02, Kle03, KB09, LMV07, LMB08, LLS03, LWH06, LHP01, LK03, LKW04, LZF⁺09, MN02, MZ05, MBWP03, MHT01, MC06, OFB08, PDC⁺08, PSMB05, Qua04, RSSKB03, RCJ02b, RK04, SAM06,

Sch03, ŠBL05, SYC03, STH02, SE08, SDL07, SSB07, TBG00, TCR⁺02, TBGRJ04, VMA03, VC04, VMF⁺03, WMGK07, WMW03, WMW04, WSM⁺08, WCL05, WM01, YLL⁺09, ZM03, vDSSvA04]. **methoxycarbonyl** [KK09]. **Methyl** [CADW03, CCK01, DBM03, DMN05, HT05, RC04, WLX⁺05, WDZS07, WSM⁺08, WLL⁺03, WC08, ZLLS05]. **methylacetamide** [MMPK01]. **methylacetylene** [ZKZ⁺07]. **methylamine** [LMB08]. **methylation** [EL07, HM08, SLC⁺09]. **methylene** [LFS⁺07]. **methylenimine** [dOMSL01]. **methylenimmonium** [dOMSL01]. **methylimidazole** [HT05]. **methyloxaziridine** [ZPL07]. **methyloxirane** [ZPL07]. **methyltransferase** [WC08]. **MF** [DHW⁺08]. **MF-3D-QSAR** [DHW⁺08]. **Mg** [WZZ⁺09, AS06, LST08, ŠBL05]. **Mg-porphin** [ŠBL05]. **mGluR1** [FTLV01]. **MgO** [SBG09b]. **MHz** [CMD⁺04]. **MICCs** [YGZZ05]. **micelles** [KS02a]. **Michael** [Ano00]. **microcanonical** [Rap06]. **Microiterations** [VMF⁺03]. **microscopic** [PK04]. **microsecond** [MST⁺08]. **microsolvation** [UM03]. **microwave** [ZGXX06]. **middle** [RPNJ07]. **migration** [HLB09, ZGZX07]. **MILCH** [BL09]. **mimic** [WMS06]. **minima** [CA04, DLD⁺02, KG02, XOW⁺00]. **Minimal** [BWZ08, BVW04, Maz01]. **minimization** [EGSG00, OM04, Sen06, WG02, vEMK01, ABF⁺03, NCO⁺05]. **minimizations** [dSR08]. **minimized** [GLD08]. **Minimum** [AM06b, AJ03, CZB07, CY09, CY13, SBLK01]. **mining** [CDD⁺02, KG02]. **minor** [BCP03]. **misfolded** [CP08, WS07]. **mispairs** [SG07a]. **mixed** [FÁ01a, HELM09, MPF00, MC06]. **mixed-valence** [HELM09]. **mixing** [AMR04]. **mixture** [WG02]. **mixtures** [FBDG06, NL07, YGLvG06]. **MLR** [HSMT04, LLL⁺08]. **MM** [CGBF05, MPF00, AST06, CR09b, CG05, FAR02, FMSA06, FSK05, GWM08, GC04, GWM⁺00, HHH00, HBM06, HNR08, HRR05, HTN03, IV04, IvSV06, ITS05, ITS06, KHF⁺09, KPR04, Kri08, Kri09b, LLL03, MBM⁺00, MK02, MSH⁺06a, MG00, MLJ03, NGTB03, PB06, RG02, SBG⁺09a, SN06, SMM⁺08, SVV⁺08, THHN01, TdMSD⁺08, VMF⁺03, WCC08, WHF08, WHG⁺07, WC08, YZ06, ZWZ09]. **MM-PB** [GC04, WHF08]. **MM-PBSA** [PB06]. **MM2** [KKY01]. **MM3** [AD00, LSWB00, YSA⁺03, FH01, Sto05, SBH02, TAS07]. **MM3/MM4** [AD00]. **MM4** [AD00, CLFA07, LLA01d, LLA03, ACLD03]. **MMPBSA** [ZWB09]. **MMVB** [GRO⁺03]. **Mn** [AZM03, BL00, GD06, BL00, PYS05]. **MNDO** [DC02, RCJ02b, TBGRJ04]. **MNDOC** [IK00]. **Mo** [LZZC09, ML00, DRAS04, DRAS05, LDMR01]. **MO/statistical** [ML00]. **mobility** [HIM07]. **MoCalc** [DPDG05]. **Modal** [ES00]. **mode** [EBAN07, HNR08, KSU03, KJP⁺07, KK01a, SFRS01, TVL⁺03]. **mode-specific** [SFRS01]. **Model** [CPML08b, Duk01, EL07, Van08, AB08, ABBC01a, ABBC01b, ATM⁺07, APG05, BG00, BBHD04, BLL⁺06, BT00, BCIB05, BB08, BLN01, Bof01, BLMS08, CFK08, CF04, CFC⁺08, CP08, CP09, CRSB03, COMR⁺04, CMGDAC⁺07, CA07b, COL01, COL⁺06, DLWV07, DHW⁺00, DAK08, EA08, EDW07, EKO⁺01, FKL⁺06, FCK⁺08, FEVM01, FC06, FBLO08, FZL⁺06, FNP⁺06, GZL02, GL04a, GK09, GJK00,

GKTS04, GGT08, GWS⁺02, HB09, HPL03, HS01, HK08c, HK08d, HHP04, ILB03, JBB00, JJB02, JPF⁺00, JBGK08, KSB⁺02, KFZ03, Lab08, LRI⁺02, LAR⁺03, LFZS04, LJ04, LSHR04, LR06, LK03, LK04, LKA01, MWL⁺08, MMPK01, MCF05, MBC08, Nak07, NL07, OKE⁺02, PCO⁺07b, PCO⁺07a, PMB04, PFC03, Pom04, Qua01, RMP01, Sen06, TJE03, TCT03, TGGP⁺00, Tot04, TT02, VW00, VW04, VGDSU08, VP09, WCK00, WKYU01]. **model** [WS05b, WEE01, WOC⁺03, WJX⁺08, XL02, XZ05, XLT07, YL09, YPNE09, YJF06, vDSSvA04, FCP⁺04b]. **modeled** [PB05, vDSSvA04]. **Modeling** [ECM⁺03, FRS05, MCR08, Mck07a, Mck07b, MTB09, PSCD⁺09, SEKS09, Sie01, BA03, BA04a, BZP09, BM08, BSH07, CLP09, ČJPZS08, DJT08, DMN05, EDAJ04, ENM⁺04, GL04a, Gor01, HBM06, HMSM06, HMMS09, HRBKB03, HP04, Hin00, JM07b, JTR05, KCL06, KS01a, KJP⁺07, KVS⁺06, KPZK06, LEK07, LLL⁺08, LFR⁺04, MMLC05, MBM⁺00, MPF00, OFB08, SPGS08, SGS03, SY⁺03, SS05, SPF⁺07, Sto05, TTBM09, VBGL⁺00, XLC08, YKK09, ZBS03, ZMH⁺09, BBC⁺05]. **modelling** [PSHP08]. **Models** [JB04, AS09, AHGK09, ACM⁺06, CCK01, CPUGD09, CRGN07, CA04, CA07a, CCT⁺03, DMN03, DLG00, DR07, DDVD09, EC06, FWH⁺07, FK07b, GSB09, GDV03, GS02, GDPCPU07, GDPP08, GS08, HdMdS05, HdS06, HD06, HP01, HLT⁺05, HG08, HJCP01, JPF⁺00, KS02a, Kr603, LJKL08, Leh06, LS08b, LDTS07, MTE04, MA05, MC06, OGH05, OYH05, PFJ⁺03, PA05, QSS01, RD06, RSP03, RSER09, RS08, RR05, SBLK01, Sch00, SSS⁺09, SRB02, SKK⁺07, SB01, SL06, VBS09, WB04a, WB04b, WB05, WZXY07, YÇBM00, YGLvG06, YJF06, YKK09, ZLJS03, ZCL09, ZGFL01, ZLD09, ZWP08, TDH06]. **Modern** [PB02, FLK⁺07, Pra01]. **modes** [Gra07, LSY02, MGLL03, OR05, Tor02]. **Modification** [HNL08, Vya01, YWH04, CM09, KFZ03]. **Modified** [LC06, NTH09, RC04, AVS09, CLA⁺00, KKY01, NA06, VVS07, WCS09]. **Modifying** [XLT07]. **Modular** [EA06]. **module** [HMD06]. **moduli** [LZZC09]. **MOF** [TAS07]. **MOF-5** [TAS07]. **Moffitt** [Kar01]. **moiety** [LBG08]. **Moldyn** [RMHK03]. **Molecular** [AS09, BBG⁺04, BG07, BDW00, CLC09, CLFA07, CCK01, DJT08, EMP07, FEVM01, FPN⁺05, GJK00, HLB09, Ish03, JTR05, KŠB09, KAS⁺07, KLB03, KIM⁺09, LLA01a, LLA01b, LLA01c, LLA01d, LLA03, LSWB00, MLA00, Maz01, MO09, MS00, MST⁺08, NBJ04, Pin01, RMP01, RRZA08, SHD⁺08, SDM02, VSW⁺03, WEE01, YSA⁺03, YGLvG06, YKK09, ZCZ03, ZWS⁺09, AM09, ARL01, AS06, AG00, ALB09, AD00, AGMPRG⁺08, ATMK03, AM06b, AB09, AGO⁺02, APG05, AS00, BG03, BP00, BR07, BA08, BB05, BWE05, BRDC02, BWZ08, BVW04, BT00, BSOB05, BME05, BSJ01, BPCD07, CMJ08, CC07, CDS09, CCL06, COS01, CW02, CIB05, CDD⁺02, CFK08, CCSJ00, CGBF05, CF06, CF04, CPC⁺00, CR02, CCP04, CEP07, CMD⁺04, CSU05, CBH⁺03, DvG00, DB07, DPT03, DFWH05, DFGB09, DPDG05]. **molecular** [DSS03, DMC05, DLHC06, DK01, DWC⁺03, ESM06, EKB02a, EKB02b, FSM09, FHRR07, FG02, FOK⁺04, FKL⁺06, FII⁺07, FÁ01a, FBDG06, FLOD07, FAB⁺00, FKZ09, FEV⁺09, FKRE08, FNP⁺06, FRLN09,

FKU⁺⁰⁵, FKM⁺⁰⁶, FKM⁺⁰⁷, GL04a, GLP08, GKRG08, GCCVB00, GLMV09, GFS05, GLD08, GRCD01, Gly06, GS02, GS03, Gon07, GSDT09, GCD⁺⁰⁸, GS04, GKTS04, GPK05, Ham07, HB09, HHWG08, HYT05, HGMB04, HH04, HELM09, HM08, HLS07, HSWN01, HN02, HP04, Hin00, HIA03, HTKG08, HK08d, HW03, HTN03, IKN08, ITS05, IC08, Ish04, IIK09, IKYM09, JS07a, JMD⁺⁰², JP09, JGVF05, JFG04, JHPRSM⁺⁰⁵, KMH02, KFZ03, KKG⁺⁰⁹, KM00, KCL06, KEB04, KKC05, KSY⁺⁰⁰, KAK⁺⁰⁹, KCK⁺⁰⁸, KBL08, Kni00, KZRO03, Kol04, KIFK07, KvGH01, KH06, KC01b, Kri09a, KPR04, Kri08, Kri09b, Kr603]. **molecular** [KKS04, LFK05, LL00, LSG06, LFSB03a, LFSB03b, LCKL05, LPK07, LJ04, LTF⁺⁰⁷, LS05a, LKT04, LM03, LPB03, LEV⁺⁰⁹, MB00, MFB04, MN02, MBP09, MM03, MABM09, Mas01a, Mas01b, MDA08, MVL⁺⁰⁵, MH08b, MG00, MCM04, MS01, MPF00, NK01, NYK⁺⁰⁹, OBBS05, OS06, OO04, OO06, OSHS03, OR05, OCP02, ON07, OO08, PMGL03, PRKP05, PMB04, PS09b, PBW⁺⁰⁵, Pin03, PWHF⁺⁰³, PWHF⁺⁰⁴, PDS01, Pog06, PTC01, PRT⁺⁰⁷, PRT⁺⁰⁸, PZS04, PPYS08, PHH⁺⁰⁸, PB02, PNG08, QTdG⁺⁰⁸, QNF09, RP07a, Rao00b, RP02, RLRE01, RLER04a, RLDI09, RSN⁺⁰², RMHK03, ROG00, RM00, RGP⁺⁰⁷, RHL09, SF07, SO07, SDL⁺⁰⁹, SH09, SBJ08, SEKS09, SBG^{+09a}, SYY⁺⁰³, STH02, Ste04, SPF⁺⁰⁷, SVT09, TJM⁺⁰³, TYN05, TLKT00, TT08, TFN04, TGGP⁺⁰⁰, TFZRG01, TCR⁺⁰², TT01, TT05, TRS02, TBGRJ04, UTH⁺⁰³]. **molecular** [UIHN09, VSK⁺⁰⁴, VW03, VCM01, VP02, VHRR07a, VHRR07b, VC04, VM00, WCF04, WZZ⁺⁰⁹, WWL⁺⁰⁹, WTKM06, WMS06, WNH03, WD08, WSC09, WRBV03, WM01, XLZ08, XOW⁺⁰⁰, YGZZ05, YXC⁺⁰⁷, YL09, YH06, YH07, YZ04, YTH⁺⁰⁷, ZMZ09, ZAT07, ZWZ09, ZSK07, vdVGDM00, BRV⁺⁰⁷, CLP09, HWTL03, LPP06, LLXS02, LGB⁺⁰⁹, MCR08]. **molecular-dynamics** [WD08]. **molecular-loop** [PRT⁺⁰⁷, PRT⁺⁰⁸]. **molecule** [ALKH04, BAL⁺⁰¹, CLP09, FM00, KK08c, MZ05, NK06, Oos09, Pin03, RGG08, SM08b, SFC04, SSW⁺⁰⁷, SVV⁺⁰⁸, WLPF05, WDS06, XDS06b, ZLLS06a]. **molecule-based** [KK08c]. **Molecules** [LLXS02, BG03, BHTCG07, BG00, BZP09, BT00, BKS02, CLP⁺⁰⁵, CG03, Che01, CRSB03, Cul08, DDKV07, DHF⁺⁰⁵, DR09, DRAS04, Eli07, EKO⁺⁰¹, FCW06, FÁ01a, FS02, FS04, GCDL⁺⁰⁵, GCD04, GBBH09, HIM07, HDF⁺⁰⁷, IS07, IC08, JVVK09, JG03, KGN07, KH01, KP05, KKG⁺⁰⁹, KLH⁺⁰⁴, KCK⁺⁰⁸, KOFF09, Kol04, KvGH01, Leh06, LZA02, LYS08, MWL⁺⁰⁸, Mat03, MSH^{+06b}, MSR04, MA09, MH08b, MBH⁺⁰², NRKH02, PO03, Pan07, PHJ⁺⁰⁸, PDS01, PPYS08, PSS⁺⁰⁴, PSMB05, RLR⁺⁰⁴, RLER04a, RLER04b, RRZA08, RZWS07, SD09, SHH07, TLOG00, TD06, Tor02, VKP⁺⁰⁸, Van02a, VM07, WCK00, WL04, Wil01b, WR07, WFR08, Wou00, YT03, YGZZ05, YK08, Yos02, ZZY07, vEMK01, vE01, vGGB00, PFB05]. **MOLFDIR** [PVdJB00]. **Møller** [CPML08a, DSR⁺⁰⁷, FII⁺⁰⁷, Gri03, IN08, JSHG07, Var09, WCFH02, YH09]. **MOLMAP** [HMMS09]. **MOLPRO** [VW03]. **molybdenum** [BGC⁺⁰⁹, SS05]. **moment** [HK08a, HK08d, HK08b]. **moments** [DVP⁺⁰², GdSuM⁺⁰⁷, MLA00, Mar03, PP08b, RP07c, VC04, YOB⁺⁰⁸].

momentum [GY08, WMRW⁺⁰¹]. **mono** [CU01, GWL07, MGMM07b, HT05]. **mono-** [CU01]. **monoanion** [Bac09]. **monochloride** [ZL05]. **monocopper** [GTC06]. **monoderivatives** [EB04]. **monofluoride** [LB08]. **monohalides** [CWWS07]. **monohydrates** [GGP09]. **monomer** [YXC⁺⁰⁷, ZM06]. **mononitrides** [Wu06]. **mononuclear** [CZ05, GK09]. **monooxygenase** [HLLN06, HYR06, TMBM02]. **monophosphate** [MRS⁺⁰⁷]. **monophosphide** [ZKZ⁺⁰⁷]. **monopole** [ZFL⁺⁰⁵]. **monoprotonated** [HA04]. **monosaccharides** [GGK⁺⁰⁸]. **monosilicide** [HXD08]. **Monosilicon** [YDWS06]. **Monosilicon-substituted** [YDWS06]. **monosubstituted** [COMR⁺⁰⁴, Lee09]. **monoxide** [GGP09, HT05, YQQH09]. **Monte** [NCO⁺⁰⁵, SCS07, AGSFAL05, AGSFA⁺⁰⁵, BR03, BHG03, Der00, FCK⁺⁰⁸, FKFG08, GHH07, HMD06, IM06, IKYM09, KLS02, KM07, KKC05, LML⁺⁰⁰, LZA02, LRWG03, MH09, Nak02, NA06, OM04, SKGS00, SBJ08, SM08b, SWR06, TS05, XKG⁺⁰⁵, ZCS04]. **Monte-Carlo** [KLS02]. **montmorillonite** [DJT08]. **MoO** [LZZC09]. **MOPED** [SRCD03]. **MORPHY** [MP03b]. **Morse** [SDCG02]. **Mössbauer** [HLLN06]. **most** [KAS⁺⁰⁷]. **motif** [HHW⁺⁰³, LLL07]. **Motifs** [HWTL03, WHH⁺⁰⁶]. **motion** [BRDC02, CCSJ00, LPK07]. **motions** [HSWN01, KS05b, LV08]. **Mott** [RDM⁺⁰⁸]. **MOVB** [MG00]. **move** [SM08b]. **moving** [CvG08]. **MP2** [WD04, BP02, EA08, FJP07, GCCVB00, GKTS04, IPN06, IPN07, JPF⁺⁰⁰, ME06, PFJ⁺⁰³, PMC⁺⁰⁸, SAM06, WD04]. **MP2/cc** [WD04]. **MP2/cc-pVTZ//MP2/6-31G**** [WD04]. **MpProp** [SKK⁺⁰⁷]. **MPSim** [CWV⁺⁰⁵]. **MRCI** [KTM02, SZW⁺⁰⁵]. **MSINDO** [BGJ01b, JGH00, JW00, NBJ04, SBG09b]. **MST** [COL01, CSB⁺⁰³, FBLO08, MBH⁺⁰²]. **MST-based** [MBH⁺⁰²]. **Mulliken** [GHBB04]. **multi** [ABWT09, SL09]. **multi-region** [ABWT09]. **multi/heavy** [SL09]. **multiatom** [SSB⁺⁰³]. **Multibaric** [OO06]. **multibody** [CPC⁺⁰⁰]. **Multicanonical** [HHHS01, SKGS00, YÇBM00, KH01, YAÇ⁺⁰²]. **multicenter** [DBS08, MS01]. **multicentered** [DWNB01, HT03, WBSR03]. **multicomponent** [ST04]. **multiconfiguration** [NUH02]. **multiconfigurational** [GD06, PJPJdPRMI07]. **multicore** [KHF⁺⁰⁹]. **Multicut** [LSHR04]. **Multicut-HDMR** [LSHR04]. **Multidimensional** [AL01, ARL01, Chu07, HP05, PC00, PFC03, RNG03]. **Multidimensionality** [FVB08]. **multiensemble** [HKMS01]. **multiexponential** [GC03]. **multifarious** [Sim07]. **multifield** [BRDC02]. **multigrid** [BB05]. **Multis isotopic** [Gor01]. **multilayer** [LJZ⁺⁰⁷, SJJ⁺⁰⁴]. **multilayered** [MR04]. **multilevel** [BHW00, HBW00, HBW01, JNV08]. **multiobjective** [CMBC08]. **Multiple** [CLF⁺⁰⁹, CLZX09, DHW⁺⁰⁸, JW06, SK09, STH02, BYQS03, CV09, Gol09, KM00, KH06, LHJ⁺⁰⁶, MST⁺⁰⁸, PAT⁺⁰⁹, STCJ08, XOW⁺⁰⁰, PYCD03]. **multiplications** [SSB⁺⁰³]. **multiply** [HT03]. **multipoint** [WS05b]. **multipolar** [DWNB01]. **multipole** [Ami00, ATMK03, BH03, CRG01, GY08, KM00, KLM⁺⁰⁹, Mar03, RP07c,

SF07, SG01, SvDS01, TFZRG01, VC04, WL09a, WBSR03, YOB⁺08, ZFL⁺05].
multipole-based [WL09a]. **multipoles** [KS01a, SKK⁺07].
multipopulation [HHJ03]. **Multireference**
 [WNH03, CWY09, DLD⁺02, HELM09, KBT03, MLL06, ME06, QTdG⁺08,
 UKNS01, UKN04, WCFH02, dSVA⁺09]. **multireference-MP2** [ME06].
Multiscale [San01, OFB08]. **multiscaling** [VTT⁺08]. **Multispecies**
 [GDPP08]. **Multistate** [JHPRSM⁺05, FSM09, MST⁺08, YFS07].
multithermal [OO06]. **mutagenesis** [MFR07]. **mutant** [DLRZ09].
mutants [GDPCPU07, MRS⁺07]. **mutase** [HHBH00]. **mutations** [HFS⁺07].
mutual [HTKG08]. **mutual-information** [HTKG08]. **MXO** [HT05].
myoglobin [AZS⁺04]. **myosin** [HSWN01].

N [GR07, JD09, KYFW07, KSN01, LS08a, LWW⁺06, Lu09, Mck07a, Mck07b,
 OS08, Sim07, TK08, WDXS06, WD08, WJX⁺08, XWXC08, YHD⁺06, ZY01,
 ZXY03, RMHK03, XZ04, ZX04, CPC⁺00, DRAS05, FJ08, FH01, HDO⁺02,
 KKH⁺07, KBL08, Lu09, LKA01, McD08, Mck07b, PFC03, RFSS06, SN00,
 SRE08, WLL01, Wil01b, WC08, WJX⁺08, ZW09, ZX09]. **N⁻** [WJX⁺08].
N-dimethyl [WJX⁺08]. **N-dimethylhydrazone** [Lu09].
N-formyl-serinamide [PFC03]. **NaCl** [PK04]. **NAMD** [PBW⁺05]. **Nano**
 [Est07]. **nanalloy** [LJS05]. **nanocomposite** [DJT08]. **nanomaterials**
 [GJL⁺08]. **nanomedicine** [PSCD⁺09]. **nanoneedles** [PSCD⁺09].
nanoparticles [CGG06, KEM08, ZWC⁺09]. **nanotube** [KK08c, XWL⁺09].
nanotubes [BG07, ZZvRSC08]. **nanowire** [KK08c]. **naphthalene**
 [CDPL09, HRG07, WL09b]. **naphthalene-like** [WL09b]. **naphthoic**
 [CMLS05]. **naphthylisoquinoline** [BMRF01]. **native**
 [BS01, yCkHmY08, DB02, MMY07, WS07, ZCL09, ZS04]. **native-like**
 [DB02]. **Natural** [FLGW00, Bac07, GS07, LZ05b, PU09, RD06]. **naturally**
 [CJW⁺09]. **Nature** [CQ04, SK08, Ang09, KSK00, PYS05]. **Nb** [WD08]. **nbo**
 [Kar01, BPC01]. **NCH** [KRLD09]. **NCN** [LD05a]. **NDDO**
 [CSB⁺03, FÁ01a]. **NDDO-based** [CSB⁺03]. **near**
 [BVW04, PABK03, YL09, ZS04]. **near-minimal-volume** [BVW04].
near-native [ZS04]. **near-neighbor** [PABK03]. **near-solute** [YL09].
Nearest [HDF⁺07, HTKG08]. **Nearest-neighbor** [HDF⁺07, HTKG08].
NEB [GF08]. **needle** [BS01]. **Negative** [BLO⁺02]. **Neglect** [Lai07].
neglected [WCF04]. **neighbor** [HDF⁺07, HTKG08, PABK03]. **neighbors**
 [RP07d]. **nematogenic** [CLP09]. **neopentyl** [YTY07]. **Nernst** [DAK08].
net [BED02]. **Network**
 [KYL03, AG03, CLC03, Gol09, GDPP08, GAS04, HMSM06, KEB04, LSY02,
 MVLG06, NINAT⁺07, SJJ⁺04, SPT⁺03, UIHN09, WX09, LMH⁺09].
network-based [GDPP08, GAS04]. **networks** [BMRDB01, BSH07,
 FCK⁺08, KVF⁺07, LJZ⁺07, PS09a, RLA01, TCSM03, VGDSU08, dVB01].
networks-based [PS09a]. **Neural**
 [GAS04, AG03, CLC03, Gol09, HMSM06, KEB04, LJZ⁺07, NINAT⁺07,
 PS09a, RLA01, SJJ⁺04, TCSM03, WX09, dVB01]. **neuronal** [SBG⁺09a].

Neutral [DWS⁺09, ASS⁺02, Bac09, CYM02, DLR⁺08, EBDPM00, FCP⁺05, MT03, OSA06, PGG06, ROG00, VM02, Wan09]. **neutrals** [LLXS02].
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, LDMR01, MR02, Mck07b, PC00, SEKS09, dOMSL01]. **NHC** [ZL⁺08]. **NHNH** [LWY⁺09]. **Ni** [Bac09, KGL07, PMM06]. **NiAt** [ZL07].
niches [TP01a]. **nickel** [Bac09, GK09, LMIF06, YQQH09]. **nicotine** [VB09].
nicotinic [GCD⁺08, SBC⁺09a]. **NiH** [ZL07]. **NiO** [SBG09b]. **niobium** [Tie09]. **NiSOD** [PMM06]. **nitrate** [CGB⁺09]. **nitrenium** [FG03]. **nitric** [JDWS06, LPP06]. **nitride** [UNM⁺01]. **nitrides** [LX07]. **nitrido** [Bac05].
nitrites [POJ01]. **nitrite** [DBS07]. **nitro** [MA05, POJ01, UTH⁺03].
nitroethane [GWM08]. **nitrogen** [BGC⁺09, LLM09, gThDjL⁺01, WC08, XLW⁺09, ZLLS04a, ZLLS05, ZWY⁺09, ZMH⁺09]. **nitrogen-containing** [LLM09]. **nitrogen-pivot** [ZWY⁺09]. **nitrogen-vacancy** [ZMH⁺09].
nitrogenase [Ano06a, Mck07b, ST06]. **nitroguanine** [JM07a].
nitromethane [LZJ03]. **nitrones** [MGG06]. **nitroxyl** [LPP06, VCM01].
NLOpredict [MMP⁺07]. **NMR** [AGI⁺07, BPC01, BRDC02, CADW03, CMD⁺04, CMA⁺08, FO04, HP05, Kle03, KBLP09, MC06, PC00, PFC03, PF06, RI07, RSER09, ZPL07]. **NO** [LDT⁺02b, PGNG03, PGRRNG03, ZLLS04b, ZLLS06b, IS03, FJ08, GBBH09, LDT⁺02a, MR02, PGNG03, RAGLL09a, XDS06a, ZLLS06a]. **Nobelium** [HdMdS05]. **noble** [SRB06]. **nodal** [HYT05]. **nodes** [Kau07]. **NOE** [AGI⁺07, PF06]. **non** [GZ07, Gon07, SVT09]. **non-bonded** [Gon07].
non-Dyson [SVT09]. **non-IPR** [GZ07]. **Nonadditive** [Don08, PMB04, ZWP08]. **nonbonded** [ASDP⁺06, ATMK03, DK01, GWM⁺00, KH06, PABK03, SF05].
nonbonding [IB04, ZTS09]. **noncentrosymmetric** [GBJ03]. **Noncollinear** [Van02b]. **Noncovalent** [Won09, JČHS07, SP05, SMV⁺09, TH02].
noncovalently [PHFC04]. **nonelectrostatic** [KF02b]. **Nonempirical** [KSK00]. **nonequilibrium** [FZL⁺06, GG09, KK08c, LF04, LFZS04, OD09, YZ04, ZFL⁺05]. **nonhybrid** [DF04]. **nonisomorphic** [CRGN07]. **Nonlinear** [RLA01, BF04, BF07, Har04, HLSH05, MMP⁺07, WCL05]. **nonlinearity** [LPK07]. **nonmetallic** [ALC08]. **nonnative** [yCkHmY08]. **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, JLHF03, NL08, TRS02, WL09b, YWHZ03, CKR08, CMBC08, GZL02, GDV03, LXW⁺09, RI08, TYO⁺02, YJF06, ZNLL07, 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, RKH03, SYC03, SL04, SWR06, SHK⁺05]. **nucleobases** [FKŠ⁺09, SBI08]. **nucleophilic** [BSB05, SSB07]. **nucleoside** [Wil01b]. **nucleosides** [SA07]. **nucleosome** [VTT⁺08]. **nucleotide** [Mak08, MSF⁺08]. **nucleotides** [XWXC08]. **nucleus** [FVB08, HdMdS05, HdS06, HD06, IKN08]. **NUCS** [SHSF05]. **nudged** [AJ03]. **number** [CDS09, HXD08, KZRO03, KZW⁺05, KH06, TGGP⁺00, WWL⁺09]. **numbered** [GYCZ04]. **numbers** [GdAcV⁺07]. **Numerical** [DLW06, LXL07, MO01, QNF09, TT08, WL04, vW06, DB07, ESP04, FMAMVK06, IO08, WL00, YK08, WG02]. **Numerov** [Bie04a, Bie04b]. **Numerov-type** [Bie04a].

O [BL00, GCCVB00, GPSP06, HYR06, ITS06, mJIZyL⁺08, KGL07, LZCC09, LMO09, Mas01a, Mas01b, NA06, Owe05, PGNG03, PGRRNG03, UCT⁺03, XWXC08, YHD⁺06, ZJM⁺07, ZY01, ZYL04, ZYL⁺08, ZXY03, Bac09, CCCJ09, DRAS05, Dib05, HM08, HDO⁺02, IS03, LC07, LW04a, LS05b, MGLL03, NyHN06, NHN06, RAGLL09a, RFSS06, SSL02, SRE08, Wil01b, YTY07, ZX09, KZY09]. **O-methylation** [HM08]. **O3LYP** [BP03]. **OB** [NA06]. **object** [CRH⁺07, FL08, MVL⁺05]. **object-oriented** [CRH⁺07, MVL⁺05]. **objective** [WG02]. **objectives** [STCJ08]. **objects** [RSN⁺02]. **observables** [MG06]. **observations** [FWH⁺07]. **observed** [VBS09]. **obtain** [BVW04]. **obtained** [HFS03, VC04, WMW03, WMW04, WHH⁺06]. **obtaining** [Bac04, YGZZ05, SK09]. **occupied** [HHWG08]. **occurring** [CJW⁺09]. **OCF** [UTM⁺02, UTT⁺04]. **OCHF** [YLW⁺08]. **OCI** [HLLS05]. **OCLO** [WLZ⁺07]. **OCO** [VM07]. **OCS** [VS02, ZGXX06]. **octahedral** [OSA06]. **octan** [BE07]. **octan-1-yloxy** [BE07]. **octanol** [COL01, CSB⁺03, Gol09, Tot04]. **octanol/water** [CSB⁺03, Tot04]. **octet** [GR07]. **Odd** [CC07, GYCZ04]. **odd-numbered** [GYCZ04]. **off** [HP01, LJKL08, XLT07]. **off-lattice** [HP01, LJKL08]. **off-plane** [XLT07]. **OH** [Dib05, Gog08, HTN03, IvSV06, LW04a, Mas01b, WLL07a, CU01, CUSS03, GAIMVB01, GCCVB00, GGLL05, HTN03, KZY09, Kle03, KBLP09, LC07, LWY⁺09, Mas01a, MGLL03, Mui05, RAGLL09a, RAGLL09b, SEKS09, UCT⁺03, WLLS04, WLL⁺07b, WyLG⁺09, YLW⁺08, YLWL09, ZYL⁺08]. **OH-initiated** [RAGLL09b]. **OH-rotamer** [KBLP09]. **OH-stretch** [Kle03]. **OH/CI** [YLW⁺08]. **OHO** [Wil01a]. **OHS** [JP09]. **olefin** [PHKG07, YXC⁺07]. **olefins** [AVB00]. **oligomeric** [EL07]. **oligomers** [BSG07, CSJ01, Der09, LFR07, SBB02, WCL05, ZOJ⁺06]. **oligopeptides** [MGJAARC00]. **Oligovalent** [KS02b]. **OLYP** [BP03]. **on-the-fly**

[KMA⁺07]. **On-the-path** [CY09, CY13]. **One** [CR09a, BG03, Bac07, Bie04a, GKRG08, KFD06, Kri09a, Lai07, LB05, ZWS⁺02]. **one-** [Lai07]. **one-dimensional** [Bie04a]. **One-electron** [CR09a, BG03, Bac07, GKRG08, KFD06, Kri09a, LB05]. **one-step** [Oos09]. **ONIOM** [BGC⁺09, MDA08, MC06, VMF⁺03, XKKL03]. **ONIOM-molecular** [MDA08]. **ONO** [FJ08]. **onto** [NK06]. **OOPSE** [MVL⁺05]. **open** [CSV⁺07, FS02, PRSMM03, LLA01a]. **Open-chain** [LLA01a]. **open-shell** [FS02]. **open-source** [CSV⁺07]. **opening** [SRE08]. **OPEP** [ÁCD⁺03]. **operating** [DFWH05]. **operation** [PCA⁺08, SYC08]. **operators** [KRM⁺02, Qua04]. **OPFMM** [CRG01]. **OPLS** [KB02, KOML08, KDSV02, MT03, POJ01, PB05, XLT07]. **OPLS-AA** [KOML08, POJ01, PB05, XLT07]. **OPLS-AA/L** [KOML08]. **OPO** [KZY09]. **Oppenheimer** [ZWZ09]. **opposite** [JSHG07]. **opsin** [RG02]. **optical** [Bou01, CZFH07, CTFC08, Hua09a, KŠB09, LC09, LFR07, MA09, SN06, TDK07, WCL05, YFR05, Zer08, ZX08]. **optics** [MMP⁺07]. **Optimal** [GFS05, ÁCD⁺03, BSP06b, 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, CMBC08, DMN03, DV02, FM00, FRLN09, GHMP03, HHH00, HLTLP09, KKG⁺09, KBA⁺04, KHF⁺09, KK01a, LJKL08, LJ04, LS05a, LJS05, MKT04, MM03, MM00, MW00, MGJAARC00, Pen06, PU09, Pul05, RK04, SCC04, SYC08, SWM04, SSMW09, SE08, SBH02, STCJ08, VMF⁺03, WS05a, WS02a, WPS02, XZZ04, YL06, YCS07, ZBS03, ZZ08, vLBBR12, WZW⁺06]. **optimizations** [IR03, PO03, RON02]. **Optimized** [KM07, VB03, VK06, BSDM04, FKFG08, LJZ⁺07, MV06, MY08b, MY08a, WTKM06, WNH03]. **optimizer** [KG02]. **optimizing** [QSS01, SRCD03]. **Orbit** [Duk01, CR08, CR09a, DXW08, KRM⁺02, KTM02, LB08, LXS08]. **Orbital** [KIM⁺09, Pen06, WM12, ALTB06, AB09, AS00, CFK08, FOK⁺04, FKL⁺06, FII⁺07, FKU⁺05, FKM⁺06, FKM⁺07, GCCVB00, GS07, HHWG08, Hir08, IKN08, IIK09, KDG⁺09, KBL08, KIFK07, LKT04, Mas01a, Mas01b, MG00, MY08b, NYK⁺09, OS06, OO08, PU09, SRE08, SSMW09, TBGRJ04, UIHN09, VM00, WPH⁺07, vLBBR12, vdVGDM00]. **orbital-based** [CFK08]. **orbital-correlation** [SRE08]. **Orbital-orthogonality** [Pen06]. **orbital-valence** [MG00]. **orbitals** [ABF⁺03, Bac07, BME05, CVVB04, EdIVR⁺03, FMSA06, GFS05, GC02, HYT05, ITN⁺05, Ish03, JHPRSM⁺05, Kau07, Kni00, LW07, MS01]. **order** [Bie04a, DSR⁺07, FS04, Gri03, IN08, JSHG07, KGN07, LAR⁺03, LS08c, May07, MO09, QTdG⁺08, Rud05a, Rud05b, Rud05c, YH09]. **ordering** [SM08a]. **organic** [ATH⁺03, BLL⁺06, BT00, CCK01, DA01, EDAJ04, EBD⁺01, Gol09, HELM09, HP04, JLHF03, JVK09, JTR05, KLH⁺04, LH02, LJZ⁺07, LMRVFH⁺09, PO03, PB04, SJJ⁺04, SYJ⁺03, TAS07, Van02a, WCK00, YGZZ05]. **organizing** [BA08, ZA07]. **organocatalytic** [WSM⁺09]. **organocopper**

[YIN03]. **organocuprate** [YIN03]. **organometallic** [Gor01, SYY⁺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, SMKM00]. **oscillator** [AB08, LLM09]. **other** [PS03, VMF⁺03]. **outer** [BF07, GAS04]. **outline** [SE08]. **overall** [LZ05a]. **overcome** [Vis02]. **overdetermined** [RI07]. **overlap** [LKW04, SGPS09]. **overview** [Sch03, Mac04]. **oxazolidones** [OY01]. **oxazoline** [XKG⁺05]. **oxidase** [BS06, JKL08, WZY04]. **oxidases** [PS03]. **oxidation** [BTP09, DRAS05, GCCVB00, GGGLL05, LB05, RAGLL09b, SS05, XPW09]. **Oxidative** [DGD⁺05, LL00, PMM06]. **oxide** [BSJ01, CFS⁺08, CCCJ09, JDWS06, JT08, LPP06, PV07, RRS06, SBB02, ZCS04]. **oxide/electrolyte** [ZCS04]. **oxides** [ZSC05, ZLLS05]. **oxidized** [CNN07, CR02]. **oxidoreductases** [CFS⁺09]. **oxidosqualene** [SGS03]. **oxo** [CN05, WJX⁺08]. **oxo-porphyrins** [CN05]. **oxocarbenium** [LSWB00]. **oxoguanine** [FPN⁺05, JM07a, Pin03]. **oxohydrocarbons** [Wil01a]. **oxoimidazoles** [JKM08]. **oxonols** [BG00]. **oxygen** [GTC06, GWM⁺00, MML⁺06, SO09, WSC09, XPW09]. **oxygen-adsorbed** [XPW09]. **oxyl** [AZM03]. **oxyl-** [AZM03]. **oxynitrides** [WD08]. **ozone** [YLZ08].

P [BAL⁺01, Gog08, KZY09, LS08a, Lip00, OS08, QB05, WZZ⁺09, ZY01, MK02, CCP04, Mit01, RPNJ07, RFSS06, Tot04, KZY09]. **P450** [AST06, HBM06, LCC09, ZAT07]. **P450-catalyzed** [AST06]. **P450nor** [LPP06]. **P450s** [OYH05]. **p8** [BRDC02]. **P_Anhar** [GBDP05]. **package** [AGSFA⁺05, BACJCT01, CSV⁺07, GSdT09, IM06, KSY⁺00, Kli01, KWK⁺00, MABM09, OTL08, PVdJB00, RMHK03]. **package-independent** [OTL08]. **packed** [AT02]. **Packing** [MM03, CM09, CA07b]. **Packmol** [MABM09]. **PAH** [Don08]. **Pair** [FK07a, FS04, GR07, HZX04, KSTC01, LBT07, MLL06, MGCA07, Nil09, PC05, RC04, SC01, SYC03, Sim07, PC07]. **pairing** [DP04, HWTL03, PC05, PC07]. **pairlist** [HH04]. **pairlist-construction** [HH04]. **pairs** [BM08, CJDK09, FZL07, KKMMS04, PABK03, ZZW09]. **pairwise** [Ano05b, CLZ⁺09, MTE04, Sha05, VP02, VZM⁺08]. **Palermo** [Van08]. **palladium** [WCW08, WCHW09]. **palladium-catalyzed** [WCW08, WCHW09]. **pancreatic** [MBC08]. **paper** [JW12, WM12]. **para** [ASDP⁺06, KC01a, ZX09]. **para-didehydropyridine** [KC01a]. **para-didehydropyridinium** [KC01a]. **para-hydrogen** [ZX09]. **paradox** [CDGS09]. **Parallel** [BWP07, DOSG06, MBWP03, TGGP⁺00, UIHN09, ASWG07, Ano05b, AGSFA⁺05, BP02, BWM⁺09, CRG01, GBDP05, GS04, GKTS04, GPK05, HHJ03, HHHS01, IS07, IPN06, IPN07, KKC05, KOFF09, KVF⁺07, MVL⁺05, MGJAARC00, NKIS02, NG04, Sha05, SPT07, TYO⁺02, TFZRG01].

Parallelization [GJK⁺06, PVdJB00, 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, JJB02, JVVK09].

parameterized [GB04]. **parameters** [AAP00, AMR04, Ano06c, ATBLS04, BBG⁺04, BSDM04, BZL05, CYM02, DB06, DDVD09, FAR02, FSFK05, FRS05, HPL03, KFNH08, KOML08, KVL⁺04, KC01b, MMY07, MSR04, MRC03, MLL⁺08b, MC06, OYH05, OMNH08, OBT09, PRKP05, RRCA08, SO09, SEKS09, SRCD03, SHD⁺08, SCF⁺09, TT05, TTB01a, VCM01, VIP⁺06, WZW⁺06, ZSK07].

Parametrization [PDS01, COL01, SBH02, WS05b]. **parametrized** [RSP03, TAS07]. **paraoxon** [ZWS⁺09]. **parent** [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, GY08, KM00, KSY⁺00, LJZ⁺07, Sha05, SJJ⁺04, SHH07, SZW⁺05]. **particles** [BCIB05, WWL⁺09]. **particularly** [BS06]. **partition** [CCK01, CSB⁺03, DP03, GLD08, Gol09, RM07, TS05].

partitioning [ÁCD⁺03, DVP⁺02, DVRP⁺03, HMSM06, RP07a, VC04, WNH03]. **path** [ABBC01a, ABBC01b, Blo04, Bof01, CY09, GF08, GWM08, JP09, Kli01, Qua01, UCT⁺03, VGB08, WLPF05, WHG⁺07, CY13]. **paths** [FG03].

pathway [LGB⁺09, WLL01]. **pathways** [AJ03, JW06, LZKT04, MAF⁺07, Qua04, RAGLL09a, RAGLL09b]. **Pattern** [DGHR02, EKB02a, EKB02b, KEB04, AGMPRG⁺08, HWDB03, dGWH01, EKB02a]. **patterns** [CGG06, Gor01]. **Pauli** [Ish03]. **PB** [GC04, WHF08].

PBCAID [QSS01]. **PBSA** [PB06]. **PbTiO** [ZXYF09]. **PC** [Ano01b, BMRDB01, HSMT04, OSHS03]. **PC-GA-ANN** [HSMT04]. **PCM** [FKL⁺06, CRSB03]. **PCs** [HS07b]. **Pd** [DGD⁺05, GBBH09]. **PDDG** [RCJ02b, TBGRJ04]. **PDDG/MNDO** [RCJ02b, TBGRJ04]. **PDDG/PM3** [RCJ02b, TBGRJ04]. **PDE7** [DD08]. **pea** [PS03]. **penicillin** [MK02].

penicillin-binding [MK02]. **penicillins** [DSS03].

pentacarbonylmanganese [PYS05]. **pentanes** [BPC01]. **PEPCAT** [OML⁺00]. **Peptide** [Adc04, DHW⁺07, HJCP01, JPF⁺00, ONHN00, PFJ⁺03, BTP09, BWE05, BSP06a, CLWL09, CSJ01, CJW⁺09, CLA⁺00, CP09, DvG00, DWNB01, GSB09, IGNH03, LHJ⁺06, LL01, MS03, MHT01, MST⁺08, OGH05, OKH⁺02, PHFC04, SDL07, Tot04, WCF04, Wil01b, YZ06, YÇBM00, ZALMG03, ZCZ03, WHP02, KVS⁺06]. **peptide/HLA** [KVS⁺06].

peptide/HLA-DQ8 [KVS⁺06]. **Peptides** [CPML08b, Van08, Ano06c, BBHD04, BCP04, BAH⁺02, CP08, DJ04, EA08, HHP04, IKYM09, LKJ⁺04, LLW02, LXL07, MM00, MC06, OML⁺00,

OYK⁺09, OO08, OM04, PCO⁺07b, PRKP05, PFC03, SJW09, WZW⁺06, YAÇ⁺02, ZW09, ZLD09, ZOJ⁺06, PCO⁺07a]. **peptidomimetics** [BAH⁺02]. **percolation** [Mei02]. **Perfect** [Wan09, OCB02]. **perfluoro** [FO04]. **perfluorosulfonate** [YSJ09]. **perform** [ME06, WCK00, WHG⁺07].

Performance
[BM00, Cul04, CA04, DMN03, FOL⁺04, JM07b, KPZK06, LLS03, RLDI09, VBS09, ZM03, AM06a, BL05, BRV⁺07, BLMS08, CCWH02, DF04, DB06, DGI⁺08, FMPS08, KWK⁺00, KEM08, KS05c, LWH06, MA09, NYTH09, SF07, SCF⁺09, Sto05, SBH02, UKN04, 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]. **peroxy** [Dib05]. **peroxynitrite** [JM07a]. **personal** [May07]. **perspective**
[KRLD09, LMGO⁺09, PBF09]. **perspectives** [Fie02]. **perturbation**
[CWY09, CPML08a, CG05, DRMD03, DSR⁺07, FII⁺07, Gri03, IN08, LKW04, MRS⁺07, NUH02, 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, FBGD06, FM00, GLMV09, JJK⁺00, JHZ09, KSB⁺02, KT08, KFNH08, KKH⁺07, LRI⁺02, Lee09, LB05, LLL03, MFB04, Mas01a, Mas01b, MM02, Mor02, POJ01, PV07, wQZsLyZ02, QNF09, RRS06, ROG00, SMGE08, SDvG01, SMKM00, TK08, TDH06, UCT⁺03, UNM⁺01, WD04, XKKL03, XKG⁺05, YQQH09, ZALMG03, ZSK07]. **phase-space**
[QNF09]. **phases** [ALC08, CLP09, LXSf08, 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]. **phenyl** [WZY04]. **phenylalaninamide**
[HJCP01]. **phenylalanine** [SMV⁺09]. **phenylene** [ASDP⁺06]. **Philippe**
[Bic09]. **phillipsites** [LST08]. **phonon** [EL09]. **phosphatase**
[AG00, FCP⁺04a, FCP⁺05]. **phosphate**
[LDY⁺08, MBL⁺00, PMM05, PHRR08]. **phosphates** [WOC⁺03]. **phosphatidylcholine** [CEP07]. **phosphine** [HT05, LL00, MGLDS00]. **phosphinine** [FLOD07]. **phosphinine-containing** [FLOD07]. **phosphinium** [LTF⁺07]. **phospho** [RGP⁺07]. **phosphodiesterase**
[XLZ08]. **phosphodiesterase-5** [XLZ08]. **phosphohistidine** [KVL⁺04]. **phosphoimidazole** [KVL⁺04]. **phosphole** [LFR07]. **phosphole-containing**
[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, LXSFO8, 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, SRCDO3]. **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]. **physio-chemical** [CDD⁺02]. **piano** [FKŠ⁺09]. **piano-stool** [FKŠ⁺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** [Gan09]. **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, IKNO8]. **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, MGCA07, SRB02, TBSM09, WMS06, ZMH⁺09]. **point-charge** [DWC⁺03, GGLR00, SRB02]. **points** [BMLV04, BAÅ07, DLD⁺02, GMA04, HQ02, MP03b]. **Poisson** [WB04a, WB05, ABWT09, BHW00, BH03, BF04, BF07, DLG00, DAK08, FOL⁺04, GPN01, GCD⁺08, GGT08, Höf05, HBW00, HBW01, KWHH07, LDG02, NYTH09, PZS04, SATO04, Vas02, VZM⁺08, WB04b, ZGFL01]. **Polanyi** [Nye07]. **polar** [BAÅ07, CYM02, CPML08a, EB04, FÁ01a, HLLN06, HSF08, JPF⁺00, PFC03, ZXYF09]. **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, KFZ03, MR04, Maz08, RP02, SL09, WL09a, YL09]. **Polarized** [EdIVR⁺03, BSOB05, OBBS05]. **poly** [ASDP⁺06, BJS01, CHA⁺07, CFD04, MGMM07b, Qua07, SBB02, ZALMG03].
poly-isothianaphthene [CFD04]. **poly-para-phenylene** [ASDP⁺06].
polyacenes [BPCD07]. **polyacetylene** [PM02]. **polyacrylates** [LZA02].
polyalcohols [KBLP09]. **polyatomic** [GGB07a, GGB07b, RLER04a].
polyatomatics [TP01b]. **polyazidocubanes** [JWB05]. **polycoordinated** [TGGP⁺00]. **polycyclic** [Bor03, CA07b, FVB08, MGMM07a, VS08].
polyenes [MW09]. **Polyethylene** [BCF⁺09]. **polyketides** [KB02].
Polymer [Mei02, BBG⁺04, CZA03, DJT08, MM07, RRZA08, YSJ09].
polymeric [Fau01, JCA⁺02]. **polymerization** [BG07, YXC⁺07]. **polymers** [CFD04, CA04, CA07a, DC02, Der09, Din00, DDBP09, HM01, LAEL01, OKE⁺02, SHH07, VIP⁺06, YYW07]. **polymorphism** [VVBV02].
polynomial [HDBD04]. **polynuclear** [HYR06, RRFC⁺03]. **polyoxoanions** [LFR⁺04]. **polypeptide** [Cri04]. **polypeptides** [CPML08a, IB04, KF02a, KF03, Nak02, VP09]. **polyphosphate** [MRC03].
polythiophene [CA07b]. **POPC** [JM07b]. **Pople** [Ano04a, EA08].
population [BLT03, BPCD07, Pul05]. **population-based** [Pul05].
populations [KBN02]. **porphin** [ŠBL05, ŠBL05]. **porphycene** [NyHN06].
porphyrazines [LS02]. **porphyrin** [AZM03, CHRL09, LPP06, NyHN06, NHN06]. **porphyrin-fullerene** [CHRL09]. **porphyrins** [CN05, LS02, LWH06]. **portable** [SH07]. **positron** [RG08]. **Possibilities** [PRDS08]. **possibility** [LMGR05, LBG08, TT05].
Possible [HIA03, OCP02, WLL01]. **post** [WW03]. **post-HF** [WW03].
posteriori [SPDS01]. **potassium** [MCR08, MHS05]. **potential** [AMR04, AE06, ABBC01a, ABBC01b, BCNs07, BL05, Bof01, BBI⁺09, DMLI05, DMC05, DLHC06, DK01, FSFK05, FKRE08, HPP00, HRBKB03, HPL03, HFSD03, IS03, IT03, JZD⁺09, LFK05, LMK01, LS08c, MMLC05, MCF05, Nak07, NG04, NMAT01, PSC⁺01, Qua01, RD06, RNG03, RHL09, RTG00, SPDS01, SS00, Sch03, SMGE08, SSS⁺09, SHH07, SG07b, SBB02, SJW09, TBSM09, TLKT00, WCC08, WL09a, WCK00, WS07, YH06, YHD⁺06, ZCS04, ZZY07, ZZY08, ZGXX06]. **potential-derived** [TBSM09].
potentials [ATM⁺07, CLC09, CPUGD09, CKW09, DB02, FAB⁺00, FNP⁺06, GK09, GBJ03, HZX04, HHHS01, HZ06a, IKYM09, KLH⁺04, KCK⁺08, KK01b, LI07, LHI09, LK03, LK04, LLW⁺09, MCF05, MWE02, OR05, PML03, RPMP03, RLER04b, SMAdV00, SPT07, VGDSU08, dSR08].
Powder [HWDB03, HHJ03, dGWH01]. **powerful** [PSDM00]. **pp** [Bic09, Lip00, Sta00]. **PQS** [BWM⁺09]. **PR** [AVS09, VVS07]. **Practical** [BMRDB01, PHR⁺05, Woo01, You11, Blo04, Sch03, SHSF05, SWZS04,

WW03]. **precalculated** [ZMZ09]. **preceding** [CSD05]. **Precise**
 [Ami00, Ara04]. **precision** [CN03, GAdGM08]. **precursors**
 [CFD03, CFD04, DJT08]. **predict** [HL08, HZ06a, HZ06b, LL07, PB06,
 PJPJdPRMI07, 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, CJDK09, DA01, ELK+09,
 FCW06, Gol09, JIK09, KLH+04, KCK+08, KEH+02, KF03, KKS04, LCC09,
 NINAT+07, OFB08, Sch00, YCW+09, YYW07, ABÅ04, BED02, CLF+09,
 CLA+00, DB06, EK06, GP06, GAS04, HEP+02, HMSM06, HG08, KZY09,
 KP05, KFNH08, KEB04, KK08b, KS08, KOFF09, KF02a, LEK07, LXW+09,
 LHP01, LLZL09, LLW+09, MSF+08, MS04, NCO+05, NLL+09, PJB+07,
 QLHL09, RGG08, TKS+01, TLKT00, Tot04, VGDSU08, WFHP01, WHP02,
 WHF08, WX09, ZHH09, AGI+07, GCD+08, KVS+06, ZCS04]. **predictions**
 [BS01, BLB09, CP08, Ruv07, Van02a, ZLD09, vEMK01, vE01]. **predictor**
 [Kol04]. **preface** [FA01b]. **preferences** [GSB09, KK09, LKJ+04]. **preferred**
 [DV02]. **preliminary** [KMH02, PMC+08]. **Preprocessing** [SHM04].
prerequisite [WHF08]. **presence** [LZA02, RAGLL09a]. **present** [GR07].
Presentation [Rud05a]. **preserving** [QNF09]. **pressure** [Car02, MTB09].
pressures [TK08]. **primary** [HB09, JIK09, KBN02]. **primitive** [MV06].
principle [GJL+08, PRS04, ZDS+05]. **principles**
 [CS01, EBL+08, GD09, HZX04, Hua09b, KK08c, MLJ03, TK08, VP08,
 WLX+05, WZZ+09, WD08, ZXYF09, ZHMW09]. **prion** [IHK09]. **priori**
 [SPDS01]. **prismatic** [WL09b]. **probabilistic** [PJB+07]. **probabilities**
 [DP04]. **probability** [CFS03, DLW06, GCDL+05, Kni00, SK09, SCS07].
probe [CVR08, DMLI05, TH02, VSW+03]. **Probing** [PAT+09, WMGK07].
problem [ABBC01a, ABBC01b, Ano06a, Bof01, CCL06, HLTL09, Qua01,
 ST06, TKH07, XOW+00]. **problem-size** [HLTL09]. **Problems**
 [You11, ABWT09, Mat03, Vis02, Woo01]. **Procacci** [Ano06b]. **procedure**
 [AM09, BR03, CA07a, DLSVY00, GP06, KBT03, RS08, SSL02, SMM+08,
 YÇBM00, Zho06]. **procedures** [GT03, HSMT04]. **process**
 [BZL05, LGB+09, ML00, Pac06]. **processes**
 [Che01, GG09, KEM08, LDTS07]. **processing** [AGI+00, AGI+07, FEV+09].
processor [LEV+09, Yas08]. **processors** [SPF+07]. **Producing** [KBN02].
product [SFR07, YLW+08, YLWL09]. **production** [YQQH09]. **products**
 [KYFW07, LZ05b]. **PROFASI** [IM06]. **profile**
 [Ber03, CCB04, CCP04, GB02, ONHN00, Zho06]. **profiles**
 [AHK02, CMBC08, OD09, YXC+07]. **program**
 [AJ03, BBM+09, BAH+02, DRMD03, GRCD01, Gly06, GM04, IS07, Kli01,
 KWK+00, MP03b, ME06, PPXP01, PRJ02, QSS01, RMHK03, SFRS01,
 SMZW05, TRS02, UIHN09, VB07, VKCK09, Zer08, BBC+05, BKS02].
programmable [Gan09]. **programming** [SPT07]. **programs**
 [CCD+05, KS08, MBP09, SH07]. **projection**
 [FS00b, GKH05, GY06, Qua04, TKN+08]. **projector** [MOP+07].

projector-augmented [MOP⁺07]. **prokaryotes** [WHH⁺06]. **prolapse** [HdMdS05, HdS06, HD06, TW03]. **proline** [BISB02, KK09]. **promising** [JRJ01]. **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, CMJ08, CDGS09, CDS09, CPDZH08, CLC09, CVR08, CZFH07, CDD⁺02, CHA⁺07, CRSB03, CTFC08, CMA⁺08, DD08, DXW08, DWNB01, DVRP⁺03, DD00, DPM09, DSS03, DHW⁺07, EM03a, EM03b, Fau01, FTLV01, GKRG08, Hua09a, HJCP01, JPF⁺00, JWB05, JT08, KHY00, KLH⁺04, KJP⁺07, KCL00, Kri09a, Kri09b, KGD06, KPZK06, KK01b, LTF⁺07, LWLS07, LC06, LFR07, LLZL09, LMRVFH⁺09, MV06, MM02, MA09, NA06, NINAT⁺07, NAT07, OBBS05, OS08, PMB04, 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, ZXYF09, ZWP08, ZX08, ZSK07, ZMH⁺09]. **properties-based** [VB09]. **property** [BAÁ07, 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, CLWL09, CLS⁺09, CIB05, CLH⁺07, CKR08, CLF⁺09, CJDK09, yCkHmY08, CRH⁺07, CPUGD09, CSRST04, DHM⁺03, DPRR05, DB06, DB02, EBAN07, FOL⁺04, FC06, FKM⁺06, FKM⁺07, GLD08, GHH07, GL04b, GC04, GDPCPU07, GdSm⁺07, GHMP03, GKK07, GZM09, GB04, HEP⁺02, HFS⁺07, HP01, HS01, HM06, HLTL09, HLM05, HLT⁺05, HZ06a, HZ06b, HG08, HW09, HP05, ILKR09, IM06, IIK09, IT03, JS07a, JMD⁺02, JIK09, KFB05, KFNH08, KLS02, KCL06, KHF⁺09, KK01a, KIFK07, KH05, KP08, LFBSK07, LHJ⁺06, LJKL08, LV08, LZKT04, LXW⁺09, LL07, LW06, MFB04, MKT04, MLG04, MH09, Mei02, MWE02, MLL08a, MHT01, MPF00, NMAT01, OFB08, OFIK09, PB06, PHR⁺05, PC00, PFC03]. **protein** [PSHP08, PMM05, PB02, PF06, PNG08, QLHL09, RI08, RSER09, RLP08, RS08, RK05, Ruv07, SHM04, SLC⁺09, SWM04, SWV⁺05, SN06, SR09, SMG09, STCJ08, SL06, TLKT00, TGD05, VW00, VW04, VGO⁺07, VGDSU08, VGGMM05, VZM⁺08, WS05a, WS07, XZZ04, XSHC06, XLC08, XWC09, Yan04, YL06, YFS07, YPNE09, Yos02, ZP03, ZGFL01, ZS04, ZZ08, ZTS09, ZM06, dSR08, HLC09, PMB04, ZZTS09]. **protein-DNA** [PSHP08]. **protein-environment** [HFS⁺07]. **protein-ligand** [LXW⁺09, RK05]. **protein-tyrosine** [AG00]. **Protein/solvent** [PMB04]. **proteinogenic** [IKYM09]. **Proteins** [LMH⁺09, AG03, Ano06c, BBHD04, BCP03, BHH⁺09, CR02, 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, PMB04, 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, XKG⁺05, ZCS04, dSGCG00]. **proton-coupled** [CXZ⁺09]. **protonated** [CPDZH08, ZDS⁺05]. **protonation** [Bac05, CG05, DHM⁺03, HP05, KYFW07, WHF08, XZ05]. **protoporphyrinogen** [WZY04]. **prototype** [Ang09, CS01, ASDP⁺06]. **prototypes** [SSS⁺09]. **proximity** [Agr03]. **pruning** [TCSM03]. **pseudo** [LL07, VDM06, XSHC06, XLC08]. **pseudo-Jahn** [VDM06]. **pseudofolding** [VGDSU08]. **pseudoknots** [DP03, DP04]. **Pseudomonas** [NYK⁺09]. **Pseudopericyclic** [LFS⁺07]. **pseudopotential** [FMAMVK06, LK03, VW03, vW06]. **pseudopotentials** [PSS⁺04, PSMB05, SMD02]. **PSI3** [CSV⁺07]. **psoralen** [NBTN04a, NBTN04b]. **Pt** [DMN05, LWK08, LF02, RD00]. **PtCl** [LF02]. **PtF** [LF02]. **PtH** [LF02]. **Pu** [Han01]. **Publisher** [Ano04a, Ano04b]. **pump** [CVR08]. **pump-probe** [CVR08]. **PUPIL** [TdMSD⁺08]. **Pure** [WG02, Rud05a, SDCG02, SCP08]. **purpose** [DGI⁺08, JGVF05, KAK⁺09]. **Putting** [MDI04]. **pVDZ** [Wib04]. **pVTZ//MP2/6** [WD04]. **PW** [EBL⁺08]. **PyFrag** [VGB08]. **pyrazine** [LWX07]. **pyrazole** [DMC05]. **pyrazoline** [LLKC06]. **pyrazolyl** [HT05]. **pyrene** [HIA03]. **pyridine** [CHA⁺07, HT05]. **pyridines** [WRP⁺06]. **pyridoxal** [LDY⁺08, PMM05]. **pyrimidine** [LWX07, XWXC08]. **pyrimidinyl** [WJX⁺08]. **pyrolysis** [KKH⁺07, XKKL03]. **pyrope** [ZWTP⁺08]. **Pyruvate** [ČJPZS08]. **pyVib** [Zer08].

Q [BS08, KWK⁺00, WHG⁺07]. **Q-Chem** [WHG⁺07, KWK⁺00]. **Q-Dock** [BS08]. **QCISD** [ZKZ⁺07]. **QCT** [DPM09]. **QM** [CGBF05, MPF00, AGK03, AST06, AB09, CR09b, CG05, FAR02, FMSA06, FSFK05, GWM08, GWM⁺00, HHHB00, HBM06, HNR08, HRR05, HT03, HTN03, IV04, IvSV06, ITS05, ITS06, KHF⁺09, KBLP09, KPR04, Kri08, Kri09b, LLL03, MBM⁺00, MK02, MSH⁺06a, MG00, MLJ03, NGTB03, RG02, SURG06, SBG⁺09a, SN06, SMM⁺08, SVV⁺08, THHN01, TdMSD⁺08, VMF⁺03, WCC08, WHG⁺07, WC08, ZWZ09]. **QM/FE** [AGK03]. **QM/MM** [CGBF05, MPF00, AST06, CR09b, CG05, FAR02, FMSA06, FSFK05, GWM08, GWM⁺00, HHHB00, HBM06, HNR08, HRR05, HTN03, IV04, IvSV06, ITS05, ITS06, KHF⁺09, KPR04, Kri08, Kri09b, MBM⁺00, MSH⁺06a, MG00, MLJ03, NGTB03, RG02, SBG⁺09a, SN06, SMM⁺08, SVV⁺08, THHN01, TdMSD⁺08, VMF⁺03, WCC08, WHG⁺07, WC08, ZWZ09]. **QM/QM** [AB09, HT03, SURG06]. **QMCF** [PHRR08]. **Qmd** [KMH02]. **Qmd-plot** [KMH02]. **QMPPF3** [DGI⁺08]. **QMQSAR** [DMLI05]. **QSAR**

[DHW⁺08, DHW⁺09, SGPS09, CGMPT⁺08, CMBC08, CRGN07, DMLI05, DMC05, GDPP08, HSMT04, HMMS09, LLL⁺08, LJZ⁺07, LSY02, MRS09, PS09a, SJJ⁺04, TCSM03, VB07, VB09, VGDSU08, XYN⁺06, ZNLL07].
QSAR-analysis [VB07]. **QSAR/QSPR** [TCSM03]. **QSPR** [CDGS09, CDS09, CDGS09, GS08, HM08, TTBM09, TCSM03, ZNLL07].
QSPR/QSAR [ZNLL07]. **QTAIM** [MGMM07b, RKA⁺09]. **quadratic** [ABBC01a, ABBC01b, Bof01, HG08, Qua01, ZHH09]. **quadrature** [CG06, DBS08, GC03]. **quadrilaterals** [GKK07]. **quadrupolar** [CMA⁺08].
quadrupole [HLLN06, HK08a, HK08b]. **quality** [BG03, CMJ08, EM03b, FKZ09, JJB00, JJB02, SSS⁺09, TSSGS07].
quantifying [GT03]. **Quantitative** [Mit01, WZY04, YNZ⁺08, BAÅ07, CDGS09, CDS09, DHW⁺08, DHW⁺09, Gra07]. **quantization** [GLMV09].
Quantum [AVB00, BWM⁺09, BISB02, BS06, DMN05, ECA06, ESM06, ED AJ04, FHRR07, LBT07, MBL⁺00, MA05, NRKH02, PM02, RM07, RON02, SC01, SS05, TLOG00, VHRR07a, ZMH⁺09, AGMPRG⁺08, AGO⁺02, APG05, ATH⁺03, AGSFAL05, AGSFA⁺05, BSJ01, BPCD07, CLP09, CDGS09, CZFH07, Con02, CKW09, COL⁺06, DBS07, DBM03, DA01, DWC⁺03, EBD⁺01, FCK⁺08, FÅ01a, FAB⁺00, FKFG08, FR06, FKU⁺05, GAIMVB01, GVATG03, Gog08, GBB07, GGLR00, GS04, HM08, HHP04, JJH01, JČHS07, KSB⁺02, KFNH08, KJVW08, KHY00, KZRO03, KLM⁺09, LX07, LHP01, MFB04, MP03a, MGCA07, MKT04, MR09, MBP09, Mat03, MC06, MPF00, 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, ZCZ03, ZAT07, ZSK07, SB08, CGBF05, DSS03, KBL08, PFB05, SCS07]. **quantum-chemical** [DA01, SFRS01, VKCK09, XYN⁺06]. **Quantum-connectivity** [EDAJ04].
QUantum-regions [SB08]. **quartet** [MSBS01]. **quartet/metal** [MSBS01].
quartets [MSBS01]. **quartic** [SAS05]. **quartz** [ZWPR⁺04]. **Quasi** [AGI⁺07, NUH02, AGI⁺00, ITN⁺05, VMA03, YH07]. **quasi-canonical** [ITN⁺05]. **Quasi-degenerate** [NUH02]. **quasi-flexible** [AGI⁺00].
quasi-relativistic [VMA03, YH07]. **Quasirelativistic** [HWFN01].
quaternary [CW02, SO07]. **quaternions** [CSD04, CSD05, Kne05]. **Quick** [LMV07]. **QUILD** [SB08]. **quinolines** [KS05c]. **quinoprotein** [JJH01].
quintet [GWL07].

R [Bof01, CPJ00, LZC09, Lip00, Qua01, ZY01, LZC09, ZPL07]. **rack** [OCP02]. **Radial** [GC03, ESP04, Kau07, Kni00]. **Radical** [XDS06a, AVB00, BL06, CUS00, CU01, CUSS03, CXZ⁺09, GSB09, HIA03, JDWS06, KOML08, KKMMS04, LC07, LMK01, NSB08, OO04, gThDjL⁺01, WDWS06, WDS06, WDZS07, WyLG⁺09, WLZ⁺07, WLL⁺03, XDS06b, YLWL09, ZLLS04a, ZLLS05, ZLLS06a, ZZL⁺09, CXZ⁺09, QZZZ03].
radical-molecule [ZLLS06a]. **radicals** [BE07, Dib05, Lee09, WLLS04, WDZS07, WSC09, YLW⁺08, YLWL09, ZM03].

radii [OCB02, PML03]. **radon** [HD06]. **Raf** [GC04]. **Ramachandran** [SDL⁺09, GSB09, HHP04, PFJ⁺03]. **Ramachandran-type** [SDL⁺09]. **Raman** [Bou01, LC09, NRKH02, OBBS05, Zer08]. **RAMSES** [BMRDB01]. **random** [CY09, CY13, CA04, HXLS09, JS07a]. **randomized** [LFKL00]. **range** [CEP07, GPK05, Gri06, HGMB04, IZA06, JPCA08, KSS08, MN02, RP07c, RLP08, San01]. **range-separated** [JPCA08]. **rank** [RP07c]. **ranked** [TBSM09]. **ranking** [KSM05]. **Rapid** [GGA00, RSN⁺02, BH03, Gra07, KMH02, KC01b, WS05a, PABK03]. **Rapidly** [KF02b, Zho06]. **rare** [LZZC09]. **Ras** [GC04]. **rate** [Chu07, GGB07a, GGB07b, JHZ09, MGLL03, NSU⁺02, SLL⁺04b, SFRS01, UCT⁺03, WLLS05, WLL⁺07b, WDX⁺02, ZP03]. **rates** [HG08, JIK09]. **Ratio** [LR06, KBB09]. **Rational** [Chi03, BSP06a, Ham07, VGGMM05]. **rationalized** [Bac05]. **rattle** [FS98, FS00a]. **raw** [RON02]. **ray** [HSWN01, HN02, WKYU01]. **Rb** [GLRL02, GWL07, HRR05]. **Re** [LJKL08]. **Re-examination** [LJKL08]. **Reaction** [CU01, JKM08, JDWS06, KKJH08, MGG06, Qua04, WCHW09, ABBC01a, ABBC01b, BAL⁺01, Bie04a, Bof01, BS03, CUSS03, CG05, DRAS04, DRAS05, FG03, GZL02, GF08, GWM08, Gog08, HLLS05, Hir08, HLSH05, HTN03, IN01, JJH01, JHZ09, LMGO⁺09, LMK01, LL01, LFZS04, LW04a, LDT⁺02a, LDT⁺02b, LWY⁺09, LLL07, MGLL03, MG00, MS04, Mui05, NSU⁺02, OON01, PGNG03, PGRNG03, Pom04, PS03, PMM06, wQZsLyZ02, QZL⁺04, Qua01, Qua07, RSN⁺02, RD00, RWBH09, R3JLR06, RR05, SLL⁺04a, SLL⁺04b, SRE08, TYN05, gThDjL⁺01, TGLL07, TMBM02, UCT⁺03, VGB08, WLL01, WDWS06, WLL⁺07b, WCW08, WHG⁺07, XDS06a, YLZ08, YQQH09, ZZL04, ZLLS04a, ZWL⁺05, ZLLS05, ZLLS06a, ZLLS06b, ZZW⁺07, ZZL⁺08, ZZL⁺09, dRLMS00]. **reaction-diffusion** [Bie04a]. **reactions** [AM07, BS03, CUS00, CFD03, Fie02, GAIMVB01, GMA04, GLH⁺08, GGB07a, GGB07b, HFHL06, HSWW00, JM07a, mJLzLyL07, mJLzLyL⁺08, JHZ09, KYFW07, KIM⁺09, LL00, LDC⁺07, MBL⁺00, NTH00, OY01, OY03, RNG03, Rao00a, RC04, RY09, Rud05b, Rud05c, Sch03, Sie01, SSB07, TT08, TCR⁺02, UNM⁺01, VBGL⁺00, WLLS04, WLLS05, WDS06, WLL07a, WyLG⁺09, WDX⁺02, WLL⁺03, XLL⁺02, XDS06b, YT04, YLW⁺08, YLWL09, ZLLS04b, ZKZ⁺07]. **Reactive** [LLM08, Hir08, MMY07]. **reactivities** [HTSR04, YIN03]. **reactivity** [Ano06a, BM08, Bor03, BL00, CN05, FZL07, GTC06, MTB09, ST06, Tie09, TSSSG08]. **reagent** [DHW⁺07]. **Real** [Woo01, You11, PBF07, PBF09, Sch04, THHN01]. **Real-World** [You11]. **rearrangement** [NSB08, PA05, ZGZX07]. **rearrangements** [LLKC06, YTY07]. **Reassessment** [DBM03]. **Reassociation** [DWNB01]. **recently** [RG08]. **RECEP** [KC01b]. **receptor** [DLRZ09, FKM⁺05, FKM⁺06, FKM⁺07, GCD⁺08, HMK02, KBK⁺01, MHL⁺09, SBG⁺09a, TFN04, TJE03, WS02b, XWC09]. **receptors** [CW02, FTLV01, NHH05, YKK09]. **ReCO** [HT05]. **Recognition** [UNHYT06, AGI⁺00, AGI⁺07, AGMPRG⁺08, BR07, CW02, DGHR02, 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, Bof01, CNN07, CP08, DLD⁺02, Ell07, GSDT09, HP01, Qua01, RS08, WEE01]. **Reduced-size** [BSOB05, OBBS05]. **Reducing** [PRSM02, SSL02, SY09]. **reductase** [CFER04, CGB⁺09, CBC⁺08, DBS07, GGLR00, HLLN06, LPP06, PCS04, PFR04a, PFR04b, TMBM02]. **reduction** [CCCJ09, DBS07, DMN05, HLTLP09, LRWG03, Mck07b]. **reductive** [PS03]. **reevaluation** [Kle03]. **Reference** [ZZ08, CF04, CFC⁺08, LZ05a, NUH02, OV03]. **Refinement** [HB09, Ruv07, BHW00, MM05]. **refinements** [GPK05]. **Refining** [CLWL09, SB01]. **refractive** [YYW07]. **regarding** [KZY09]. **region** [ABWT09, Ama02a, HHH00, WEE01]. **Regional** [TKH03, NTH09]. **regions** [HYT05, SB08]. **regioselectivity** [AVB00]. **Registering** [GBL⁺05]. **regression** [DLWV07, Gol09, GS08, LCC09, SY09]. **Rehybridization** [AM07]. **related** [ALC08, ACLD03, CFD04, KC01a, LXW⁺09, LWH06, LCDA03, LCGA03, LCA03, ML00]. **Relation** [SM08a, DVRP⁺03]. **relationship** [DHW⁺08, DHW⁺09, JPCA08, KWK⁺01, WLX⁺05, KWK⁺02]. **relationships** [BAÅ07, CDGS09, CDS09, CPUGD09, JLHF03, PSCD⁺09, WZY04]. **Relative** [SWV⁺05, BLB09, CG05, MML⁺06, MRS⁺07, RSE07, ZOJ⁺06]. **Relativistic** [FHF⁺01, NYH02, NSO⁺07, SNM⁺06, SMD02, WTKM06, YH09, ASS⁺02, BBI⁺09, Dya02, GHLK⁺02, GPSP06, HdMdS05, HdS06, HD06, LF02, SH02, Van02b, VMA03, WL02, YH07]. **relax** [GFS05]. **relaxation** [BRDC02, HS01]. **relaxed** [AEE⁺03, CA07a]. **relevance** [Ano06a, MGCA07, ST06]. **reliability** [IB04, LKW04]. **reliable** [BE06, WHF08]. **remove** [LZ05a]. **removing** [PCS04]. **reordering** [TVL⁺03]. **reorganization** [FZL⁺06, KMM07]. **repair** [Pin03]. **reparameterization** [RFSS06]. **repeat** [NK01, NL08]. **Repeated** [KH01]. **Repeated-annealing** [KH01]. **replica** [FSM09, FGR07, GLP08, NCO⁺05]. **replica-exchange** [FGR07, NCO⁺05]. **Reply** [Bof01, CPML08b, WM12, CSD05]. **Representation** [GPK05, BB08, CKR08, CF06, JIK09, LW04b, LXZ06, LW06, RLR⁺04, WEE01, hYDN⁺08]. **representations** [BMLV04, LAR⁺03, LR06, RS08, SN00, YNW05]. **representative** [YLL⁺09, YXL⁺09]. **reproduce** [VBS09, WS05b]. **reproducing** [MFB04]. **repulsion** [COL⁺06, Kri09a]. **repulsions** [HGMB04, PBF09]. **repulsive** [BDW00, CFC⁺08]. **requirements** [AM06b]. **research** [JLHF03, PGH⁺04]. **residual** [RI08]. **residue** [MH09, NBTN04b, PMM06, NBTN04a]. **residues** [CFS⁺09, DHW⁺07, HJCP01, JPF⁺00, OS06, UNHYT06, XLT07]. **resolution** [BS05, BS08, CDGS09, DSR⁺07, GL04a, HXLS09, Nee03,

WMRW⁺⁰¹, WS02b]. **resolution-of-the-identity** [DSR⁺⁰⁷]. **resonance** [BM07, FLGW00, MAF⁺⁰⁷, WZXY07]. **resonances** [LMB08, PF06]. **RESP** [WCK00]. **respect** [QCK01, QCK02]. **response** [HG08, OFIK09, vGGB00]. **Restrained** [SRB02, WCK00]. **restraint** [LI07, LHI09]. **restraints** [BS08, HWTL03]. **restricted** [BdPRMAI00]. **restrictions** [KŠB09]. **results** [CSD05, LKT04, PFJ⁺⁰³]. **Retardation** [HP04]. **retention** [RC04]. **reticulum** [HLB09]. **retinal** [BL05, LFE_dL06, MSH^{+06a}]. **Retrieval** [CVR08]. **reuptake** [FPG⁺⁰⁶]. **reveal** [DLRZ09]. **revealed** [HW09]. **reveals** [Pin01]. **reverse** [AJNG01, ML00]. **Reversible** [DvG00, Kol04, NHN06]. **Review** [Bic09, CvG08, Lip00, Sta00, Woo01]. **Reviews** [LB99, Sta00]. **Revised** [ATM⁺⁰⁷, SBB02]. **revisited** [ASY01, CVVB04, PCS04]. **Revisiting** [GPSP06, JPCA08, LN01]. **Rg** [ZXY03, ZXY03]. **RGF** [HQ02]. **rhenuim** [SBH02]. **RHF** [EA08, JPF⁺⁰⁰]. **rhodamine** [VSW⁺⁰³]. **rhodium** [GLH⁺⁰⁸, LL00]. **rhodium-catalyzed** [GLH⁺⁰⁸]. **Rhodopseudomonas** [IN01, OON01]. **rhodopsin** [CEP07, YKK09]. **rhodopsin-** [YKK09]. **ribonuclease** [KSK00, WOC⁺⁰³]. **Ribonucleotide** [CFER04, HLLN06, PCS04, PFR04a, PFR04b, TMBM02]. **ribose** [SA07]. **ribosomal** [SB01]. **ribozymes** [MMMY07]. **rich** [CZ05, LWK08]. **Rigid** [SM03, DPRR05, Din00, ECA06, FS98, FS00a, Ike04, Leh06, LV08, KP05]. **Rigid-body** [SM03, Ike04]. **Ring** [ZSE08, BE09, CDPL09, DC02, DLSVY00, FJ08, RPNJ07, SRE08, ZW09]. **ring-structured** [DC02]. **RISM** [MH08b]. **rival** [DDVD09]. **RM1** [FBLO08, RFSS06]. **RMSD** [Kne05, CSD04]. **Rn** [Wei08]. **RNA** [AM06b, DW08, GdAcV⁺⁰⁷, LhWX07, LCSZ09, LOL⁺⁰⁸, MB00, Mak08, RTG00, SB01, YNW05, ZZTS09]. **RNA-ligand** [AM06b]. **RNACluster** [LOL⁺⁰⁸]. **RNase** [RWBH09]. **ro** [LN01]. **ro-vibrational** [LN01]. **robust** [GS08, HEP⁺⁰², YK00]. **ROCR** [CPJ00]. **rod** [BCIB05]. **rod-like** [BCIB05]. **Role** [BCF⁺⁰⁹, CPJ01, CFS⁺⁰⁹, CPFL02, Ruv07, SVV⁺⁰⁸, ZSC05, BY06, CDS09, CFER04, Kau07, TFZRG01, VBGL⁺⁰⁰, YT04, YTY07, YJF06, PMM06]. **Roles** [ALC08, IN01, NYK⁺⁰⁹]. **roll** [FS98, FS00a]. **room** [TD08]. **Roothaan** [TW03]. **roots** [BdPRMAI00, Nil09]. **Rotamer** [HLTLP09, GHMP03, KBLP09, LFBSK07, SMG09]. **Rotamers** [LMH⁺⁰⁹, SHM04]. **rotation** [CMLS05, COMR⁺⁰⁴, DHF⁺⁰⁵, DBM03, HFSD03, HK08c, LHI09, LZ05a, MGLL03, OMNH08, PBF09]. **Rotational** [CSD05, BVW04, KBN02, TS05]. **rotations** [IR03]. **rotors** [WR07, WFR08]. **rough** [Pan07]. **rough/fractal** [Pan07]. **roughness** [PHJ⁺⁰⁸]. **routes** [GGLL05]. **routine** [Kli01]. **routines** [AT02]. **row** [AD00, BP03, BGJ01b, JGH00, LK03, LK04, RRP⁺⁰¹, YTH01]. **Royal** [LWW⁺⁰⁶]. **RS** [LAR⁺⁰³, EK06, ELK⁺⁰⁹, KEH⁺⁰², LRWG03]. **RS-HDMR** [LRWG03]. **RT** [TYO⁺⁰²]. **Ru** [ZWS⁺⁰²]. **rule** [GR07]. **rules** [AMR04]. **runs** [EL07]. **ruthenium** [FKŠ⁺⁰⁹, PHKG07]. **Rydberg** [PRSMV08, ZM03, dSVA⁺⁰⁹].

S [BSB05, Bic09, Gog08, HKHN08, JJK⁺00, KYFW07, MGLL03, Mck07a, Mck07b, WWS07, ZJM⁺07, ZY01, XZ04, ZALMG03, DLD⁺02, HTN03, MVLG06, MG00, RC04, RFSS06, SN00, WDS06, YT04]. **S-network** [MVLG06]. **s-tetrazine** [XZ04]. **SA** [GC04, GWS⁺02, WHF08]. **SAAP** [IT03, IT03, IKYM09]. **SAC** [DHM⁺03, HFS⁺07, HKHN08]. **SAC/SAC** [DHM⁺03]. **saddle** [DLD⁺02, GMA04, HQ02]. **SAFE_p** [AVS09, VVS07]. **Sakurai** [TKN⁺08]. **Sakurai-Sugiura** [TKN⁺08]. **salts** [JHMB⁺09, KWK⁺01, KWK⁺02, JHMB⁺11]. **Salveti** [IKN08]. **Salveti-type** [IKN08]. **SAM** [WC08]. **SAM-dependent** [WC08]. **Sammon** [FKZ09]. **sampled** [IZA06]. **Sampling** [LZKT04, BHG03, CN03, CIB05, CY09, CY13, CV09, CvG08, CEP07, DDVD09, FKZ09, GT03, HKMS01, IS03, JW06, KH01, KM07, LKW04, Mak08, MH08b, MST⁺08, Nak02, NA06, RNG03, Rap06, SD09, SMG09, TS05, YL06, ZA07]. **sandwich** [JD09, 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, Ano05b, KKC05, Sha05, VGO⁺07]. **scalar** [GPSP06, KBLP09, MP03b]. **scale** [DMN03, JO02, KK01a, MH09, MHW04, MPF00, ME06, Nak02, NA06, RRS07, SSL02, TYO⁺02, WCF04, WS07]. **scale-transformed** [Nak02, NA06]. **scaled** [CN03, JSHG07]. **scaling** [AL01, ARL01, Con02, FR06, GGLR00, GY06, KLM⁺09, LMJ02, OS06, RS05, SSB⁺03, SHSF05, SKDO08, SP05, TCR⁺02, ZWZ09, vGGB00, vdVGDM00]. **scanning** [HMK02, MFR07, SMGE08, ZM06]. **scattering** [BACJCT01, Est07, HSWN01, RMHK03, WKYU01]. **SCC** [ECM⁺03]. **SCC-DFTB** [ECM⁺03]. **SCF** [JHPRSM⁺05, PFJ⁺03, PVdJB00, SAM06, VZVG06]. **SCH** [ZZW⁺07]. **scheme** [Bac04, FOK⁺04, IS03, JCA⁺02, JVK09, LMV07, Maz08, MSH⁺06b, RKA⁺09, SN00, SHH07, WS05b]. **schemes** [Bac04, Bac05, Bac07, PRS04, SPDS01]. **Schleyer** [Lip00]. **SCI** [TY03]. **SCMP** [FÁ01a]. **SCMP-NDDO** [FÁ01a]. **ScO** [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, LZ05b, PRDS08, SHSF05, YOB⁺08]. **SCRf** [CCT⁺03]. **SCUD** [LZ05a]. **ScX** [WWS07]. **SD** [WLLS05]. **SDCI** [BMB07, PRSMM02, PRSMM03]. **Se** [HKHN08, JJK⁺00, WWS07]. **search** [AM09, BR07, BMTSC01, CSJ01, CA04, GLD08, HHG⁺09, HXLS09, HM06, IZA06, KK01a, LFKL00, MGJAARC00, NL08, OGH05, OM04, Pul05, RHL09, Sau04, SE07, SE08, WK01, ZZ08]. **searches** [CZB07, YXL⁺09]. **Searching** [SPT07, STC⁺08, CvG08, Nak02, OYH09, SCC04, SYC08, YCS07]. **Second** [BC06, FS04, MO01, AGK03, DSR⁺07, DOSG06, FO08, IN08, JSHG07, LK04, QTdG⁺08, QCK01, QCK02, Rud05a, Rud05b, Rud05c, YTH01, YH09]. **second-** [LK04, Rud05a, Rud05b, Rud05c, YTH01]. **Second-order** [FS04, DSR⁺07, IN08, JSHG07, QTdG⁺08, Rud05c, YH09]. **secondary**

[CLC03, CLA⁺00, DW08, DP03, GdAcV⁺07, IGNH03, LhWX07, LCSZ09, LW06, LOL⁺08, LLL07, MHT01, WPH⁺07, YNW05]. **Section** [Ano01c, Ano04b]. **sections** [MY08b, MY08a]. **seedling** [PS03]. **segment** [YS00]. **segmented** [CGSdST06]. **segments** [BTLP03, GAS04, KF02a, YMT04]. **segregation** [Sza08]. **Selected** [BMB07, LSAS01, Mat03, PRSMM02, ZOJ⁺06]. **Selecting** [HXL09]. **selection** [HW09]. **Selective** [TCSM03, XPW09, AM06b, MHL⁺09]. **selectivity** [BSP06b, GLRL02, OO08, ZZvRSC08]. **Self** [ZA07, BA08, BWI⁺02, ECM⁺03, NUH02, NTH09, NL08, SH07, TKH03, VTT⁺08, WM04, XL02]. **self-associative** [NL08]. **self-consistent** [BWI⁺02, NUH02, VTT⁺08, WM04, XL02]. **self-contained** [SH07]. **self-interaction** [NTH09, TKH03]. **Self-organizing** [ZA07, BA08]. **semi** [BBHD04, UKN04, ZNLL07]. **semi-** [UKN04]. **semi-empirical** [ZNLL07]. **semi-implicit** [BBHD04]. **Semiautomatic** [PRJ02]. **semibullvalenes*** [HWGB01]. **semiclassical** [KM07]. **semicore** [HZ09]. **semidirect** [MBWP03]. **Semiempirical** [Gri06, LKT04, TT01, BUMCMRL00, BM00, Der09, DMLI05, FBLO08, FO08, GGLR00, HMOG07, IK00, JFG04, KSS08, KBT03, LMMW04, MAF⁺07, MSH⁺06b, MHT01, Nye07, RSKB03, RCJ02a, RCJ02b, ŠBL05, TCR⁺02, TBGRJ04, vdVGDM00]. **semiempirical-DFT** [Der09]. **Semiglobal** [DV02]. **semimicroscopic** [KK08b]. **semirigid** [CLP⁺05]. **sensitivity** [HLSH05]. **sensitization** [Sha02]. **sensitized** [KS05c]. **sensors** [BBG⁺04]. **Separable** [EA06]. **separated** [JPCA08, MLL06, WSM⁺09]. **separating** [CN03]. **separation** [FBDG06]. **sequence** [AM06b, CCWH02, CKR08, CLZX09, Dya02, JIK09, LXZ06, LSW⁺01, PRJ02, WHH⁺06, ZLY07]. **sequence-dependent** [LSW⁺01]. **sequence-specific** [PRJ02]. **sequences** [CP09, DLW06, DLWV07, Der00, JIK09, LW04b, LD05b, LW06, MCF07, PP08a, hYDN⁺08]. **sequential** [TT05, ZGZX07]. **SER** [JPF⁺00]. **serially** [KMA⁺07]. **series** [CC07, KMH02, PDS01]. **serinamide** [PFC03]. **serine** [OBT09]. **serotonin** [HLC09]. **serve** [Mck07a]. **set** [ABF⁺03, ALKH04, AHK02, BR04, BT00, BSOB05, BRV⁺07, BRLS08, BRLS12, CMJ08, Che01, DMZT08, EL09, EKB02a, FZL07, FMPS08, GGT08, HdMdS05, HMSM06, IO08, JJK⁺00, LFK05, MV06, Mas04, MLL⁺08b, MC06, PSC⁺01, PRKP05, Pen06, PFJ⁺03, PSMB05, RRP⁺01, SSB⁺03, SHK⁺05, TW03, VKP⁺08, Var09, VKCK09, WMGK07, Wib04, WG02, ZWPR⁺04]. **set-up** [GGT08]. **sets** [BY06, BSOB05, CRS05, Cul04, EA08, EdIVR⁺03, GKH05, HdS06, HD06, IO08, KK08a, LST08, LTV08, MV06, NSO⁺07, OBBS05, OVMV04, RLA01, RLRE01, RLER07, SNM⁺06, VB03, WTKM06, Wei08]. **setting** [HP04]. **setup** [ZAT07]. **several** [KS05b, XLT07]. **sevoflurane** [TZX01a, TZX01b]. **SG** [CG06]. **SG-0** [CG06]. **SGB** [GZL02]. **SGB/NP** [GZL02]. **SH** [Mas01b, MGLL03, Mui05, SSS⁺09, WLLS05]. **SH/** [SSS⁺09]. **SH3** [IGNH03]. **Shaik** [Bic09]. **shake** [KFD06, BL09, FS98, FS00a, KvGH01]. **shake-up** [KFD06]. **Sham** [Bou00, RRS07, SH02]. **Shannon** [LM03]. **shape**

[BR07, PRDS08, WM06]. **shape-based** [PRDS08]. **shaped** [LWW⁺06]. **Shapelets** [PRDS08]. **shapes** [BR07, KS02a]. **shaping** [HJCP01]. **shared** [Sim07]. **sharing** [BRS07, RS07a, RS07b]. **SHARPEN** [LMH⁺09]. **Shaw** [Ano05b]. **sheet** [KF03, PP08a]. **sheets** [LLW02, PGC05]. **shell** [DSB⁺02, FS02, FO08, HB09, PRSMM03]. **shielding** [CDL06, CDPL09, HWFN01, MC06, PFC03, WZXY07, ZPL07, ZXY08, ZLD09]. **shift** [Dra00, HP05, LFZS04, MA05, RG02, WPS02, XZ04, ZFL⁺05]. **shifted** [McD08]. **shifting** [CPFL02, HRG07]. **shifts** [CPDZH08, FVB08, FHF⁺01, FO04, HWFN01, HLLN06, Kle03, KKS04, LFS⁺07, LKA01, VBS09, WFHP01, WHP02, WZXY07]. **SHOP** [YXC⁺07]. **SHOP-type** [YXC⁺07]. **Short** [TYN05, GPK05, HGMB04, IKYM09]. **short-range** [GPK05, HGMB04]. **Short-time** [TYN05]. **shorter** [MST⁺08]. **Si** [BSB05, TK08, WZZ⁺09, YHD⁺06, CJS⁺03, SURG06, WL09b]. **sialic** [UNHYT06]. **SIBFA** [PWHF⁺03, PWHF⁺04, ROG00]. **SIBFA-LF** [PWHF⁺03, PWHF⁺04]. **side** [DLHC06, ENM⁺04, GT03, HFHL06, JPF⁺00, KG02, LL01, MT03, MMLC05, PFC03, SMG09, VM02, XLT07, ZM06]. **side-chain** [ENM⁺04, GT03, JPF⁺00, KG02, MT03, PFC03]. **sieve** [PHH⁺08]. **sieves** [LMV07]. **SiF** [LAT05]. **sigma** [JFG04, KMM07]. **sigmatropic** [LLKC06, LFS⁺07]. **SiH** [ZZL⁺09]. **silastannation** [WCHW09]. **SiLi** [XFF06, HXD08]. **silica** [SDCG02]. **siliceous** [LST08, LTV08]. **silico** [LLW⁺09, MHW04, PHR⁺05]. **silicon** [BSB05, HXD08, KZW⁺05, KS01b, LB08, NBJ04, ZLJS03]. **silsesquioxanes** [JW00]. **silyl** [MGG06]. **silylenoid** [XFF06]. **SiMe** [XFF06]. **similar** [BR07]. **similarities** [HPP00]. **Similarity** [Leh06, LhWX07, ARL01, BPCD07, COS01, Con02, HM08, MBH⁺02, PDS01, RSS09, YNW05, hYDN⁺08, ZZTS09, dGWH01]. **similarity-based** [RSS09]. **similarity/dissimilarity** [hYDN⁺08]. **Simple** [MO01, Ste04, ACLD03, Bac04, BLMS08, GRO⁺03, GDV03, Gon07, ILB03, IT03, KS02a, LLW⁺09, MCF05, SF05, BG00]. **simplex** [DV02, MCF05]. **simplex-annealing** [MCF05]. **simplified** [OYH05, WOC⁺03]. **simulate** [LAEL01]. **simulated** [ADM⁺06, AB08, CCP04, HPP00, RLP08, WM06, WG02]. **Simulating** [Fie02]. **Simulation** [FBGD06, WWL⁺09, BBHD04, BVW04, BG07, BBM⁺09, CCD⁺05, CV09, CHB⁺05, Dra00, EA06, EMP07, FHRR07, FEV⁺09, FPN⁺05, GS02, GJK00, HN02, HLB09, ITS05, IM06, IKYM09, JO02, JGVF05, KSY⁺00, KB09, KEM08, KPR04, Kri09b, LMCD09, LEV⁺09, MLG04, MMY07, MVL⁺05, MLCD01, MST⁺08, ON07, OBT09, Pin01, PHH⁺08, SO07, SL06, SDL07, TYN05, VHRR07b, WEE01, XKG⁺05, YAÇ⁺02, YTH⁺07, ZALMG03, ZWTP⁺08, ZL09b, ZSK07, OBBS05].

Simulations [FCP⁺05, MZL08, ATMK03, Ano06c, BWE05, BRDC02, Bie04b, BSJ01, CLP09, CLWL09, CLC09, CCSJ00, CF06, CPC⁺00, CEP07, CMD⁺04, CBH⁺03, DHF⁺05, DLRZ09, DFGB09, Der00, DSS03, DWC⁺03, ESM06, FGR07, FG02, FCP⁺04a, FAB⁺00, FC06, FKZ09, GL04a, GLP08, GWM08,

GHH07, GS03, Gon07, Haf08, HB09, HGMB04, HHHS01, HH04, HM02, HPL03, Hin00, HFSD03, HTKG08, HTSR04, HTN03, HMD06, IC08, JNV08, JCL05, JZD⁺09, KMH02, KFZ03, KM00, KKC05, KAK⁺09, KvGH01, KH06, Kri08, Kr603, KBN02, LML⁺00, LSO04, LGB⁺09, LM03, LPB03, MB00, MFB04, MN02, MABM09, MBC08, MO09, MG00, NK01, NL07, Nil09, OO06, 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, XWL⁺09, ZZvRSC08, Mak08]. **single-family** [WTKM06]. **Single-nucleotide** [Mak08]. **single-sphere** [LFZS04]. **Single-step** [OV03]. **single-walled** [XWL⁺09, ZZvRSC08]. **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, SPT⁺03, SFR07, TDH06, XLZ08]. **sites** [APG05, BSP06b, BSDM04, CLXC02, CLS⁺09, DV02, FPN⁺05, FSS00, GDV03, HM02, HN02, HLT⁺05, MHJS06, PPXP01, SEKS09, SLC⁺09, Tie09, Wou00]. **six** [GJK00, NL07]. **six-site** [GJK00, NL07]. **sixth** [CGB⁺09]. **sizable** [CAG07]. **size** [BSOB05, EL09, HLTLP09, KS02a, KH06, NK06, OBBS05, OV03, YAÇ⁺02]. **sized** [SHH07]. **Slater** [CVVB04, EdIVR⁺03, GC02, KDG⁺09, RLER04a, VB03]. **Slater-type** [CVVB04, EdIVR⁺03, GC02, KDG⁺09, VB03]. **slave** [FR06]. **small** [CN03, Che01, CG06, FM00, IME02, IO08, JARM02, KvGH01, Leh06, LZA02, Oos09, PO03, PBZ00, PDS01, RRS09, RZWS07, SHH07, 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, YSJ09]. **SODOCK** [CLH⁺07]. **Soft** [yCkHmY08, ASDP⁺06, TLKT00, TJE03, TGGP⁺00]. **soft-core** [TLKT00, TJE03]. **Software** [Ano04b, BACJCT01, DvL01, Gly06, JVVK09, CHB⁺05, GBDP05, KBA⁺04, MMP⁺07, NSU⁺02, BLMS08]. **solar** [KS05c]. **solid** [CFS⁺08, CCCJ09, CMA⁺08, EGSG00, Ish02, KCK⁺08, SK05]. **solid-state** [CMA⁺08]. **Solids** [vDSSvA04, JB04]. **solubilities** [SHH07]. **solubility** [BBG⁺04, EDAJ04, KEH⁺02, LLW⁺09]. **solute** [BRLS08, BRLS12, FCP⁺05, LFZS04, MR04, YL09, ZSK07]. **solutes** [BLL⁺06, HMSM06]. **solution** [ABWT09, BHW00, BP07, BISB02, BH03, CPJ00, CCK01, CRSB03, DA01, EK06, ELK⁺09, FHRR07, FG02, GMA04, HHJ03, HMWC03, HSWN01,

HRR05, HBW00, HBW01, HDO⁺02, KPR04, Kri08, Kri09b, KBN02, LRI⁺02, LXSf08, LMIF06, MB00, MH08b, PDP02, PTC01, PHRR08, RNG03, RRZA08, SH09, SATO04, SBB02, TDH06, Vas02, VBS09, YH06].

solution-phase [TDH06]. **solutions**

[Blo04, CPJ01, Loe03, PK04, VP09, XZ04, XZ05, ZWP08, LR03b]. **solvated** [HTSR04, HRR05, KHY00, QSS01, RSP03, BSC⁺01]. **Solvation**

[COL01, HHP04, WB04a, WB04b, WB05, WD04, BCIB05, CRSB03, CCT⁺03, COL⁺06, DV02, DHW⁺00, FOL⁺04, FBLO08, FZL⁺06, GS02, GS03, GPN01, GWS⁺02, HC08, HLMR06, IV04, IvSV06, KIM⁺09, LF04, LFZS04, LS08b, MGLO03, OVMV04, PZS04, PPYS08, RSE07, RP04, Sch00, SDL07, VM02, VP09, XL02, ZFL⁺05, ZFL⁺05]. **solvation-effect** [SDL07].

solvatochromatic [XZ04]. **solve** [KvGH01, XOW⁺00, Zho06]. **Solvent**

[BA03, BA04b, SMAv00, ZP03, ZGFL01, AG03, BHW00, BBHD04, BMLV04, BRLS08, BRLS12, ENM⁺04, FEVM01, FC06, GZL02, GL04a, GP06, GB04, HHS⁺05, HN02, JS07a, JZD⁺09, KIFK07, Kr603, KKS04, Lab08, LRI⁺02, LFBSK07, LSO04, 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, ZX04, ZCL09, BA04a, FZL⁺06]. **solvent-accessible**

[BHW00, BMLV04, HHS⁺05, TSMNG01]. **solvents** [GS03, IT03, THHN01].

Solving [FS00b, Höf05, BF04, CCL06, CF04, LMJ02, SATO04]. **Some**

[VE09, FMPS08, 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, BMTSC01, CSJ01, CvG08, CKT⁺08, CZA03, GT03, HXLS09, JO02, KF08, LCKL05, LJKL08, Nak02, NA06, OFIK09, PHR⁺05, PBF07, PBF09, PRSMM02, QNF09, Sch04, THHN01, Van02a, YL06]. **spaces**

[JHPRSM⁺05, PRSMM02, PRT⁺07, PRT⁺08, RSS09]. **spacing** [ZZvRSC08].

spanning [SN00]. **Sparkle** [FRS05]. **Sparkle/AM1** [FRS05]. **Sparse**

[SSB⁺03, AGSFAL05, LEK07, RS05, RRS07]. **sparsity** [JSHG07]. **spatial**

[Bie04a, Bie04b, RP07b]. **special** [KAK⁺09]. **specialized** [Höf05]. **species**

[CFC⁺08, DR09, GHLK⁺02, HBM06, KZY09, WG02, YIN03, LMGR05].

Specific [FAR02, LR03a, BS08, HLT⁺05, Pin01, PRJ02, SFRS01, TGLL07,

TST⁺08, UIHN09, WCF04]. **specificities** [PB06]. **specificity**

[CJW⁺09, DLRZ09, LLL07]. **specified** [Fau01]. **spectra**

[Bac09, BACJCT01, CNN07, CG08, Gor01, HKHN08, JARM02, KŠB09,

KFD06, LDL⁺09, MLCD01, NRKH02, OBBS05, OKE⁺02, ŠBL05, SN06,

TDH06, WM01, YXZ⁺04, ZGXX06, ZWTP⁺08, dGWH01]. **Spectral** [II02,

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

spectrometric [KZW⁺05]. **spectroscopic** [Ano06a, FCW06, KCL00, ST06].

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

spectrum [EL09, LMCD09, MWL⁺08, MGLDS00, PRSMM03]. **Speeding**

[KVF⁺07]. **speedup** [BYQS03]. **sphere**

[HdMdS05, HdS06, HD06, LFZS04, SFR07]. **spherical** [BCIB05, ZFL⁺05].

spheriphane [CS01]. **SPICKER** [ZS04]. **Spin**
 [Duk01, HYR06, KTM02, LXSFO8, 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, LXSFO8, CR08, CR09a, DXW08, KRM⁺02, LB08]. **Spinor** [PV03].
spins [JD09]. **Spiro** [HELM09]. **spiroquinazolinones** [DD08]. **spline**
 [ALKH04]. **splines** [GL04b]. **split** [EA08]. **split-valence** [EA08]. **splitting**
 [PSDM00]. **splittings** [HLLN06, SFRS01]. **Spontaneous** [Sza08]. **square**
 [CSB08, LLZL09, Nil09]. **square-planar** [CSB08]. **squares** [CSD05, Gol09].
Sr [WD08, SCP08, XB08]. **Sr-doped** [SCP08]. **Src** [OO08]. **SrFeO**
 [Hua09b]. **SrZrO** [SM06]. **SSB** [KVS⁺06]. **st2nmr** [PRJ02]. **stabilities**
 [ACM⁺06, CTFC08, GYCZ04, STC⁺08, WDXS06]. **Stability**
 [JD09, Owe05, PHFC04, WSC09, CJS⁺03, CF06, DB07, HXD08, JS07b,
 JBGK08, OCP02, PGC05, QB05, XFF06, ZXYF09, ZOJ⁺06, ZM06].
Stabilization [EBDPM00, HYA02]. **stabilized** [HSF08]. **stabilizing** [GZ07].
Stable [HDO⁺02, GDPCPU07, KYFW07, KZY09, KAS⁺07, Kol04, LMO09,
 PP08a, PZS04, STC⁺08]. **stable/nonstable** [GDPCPU07]. **stacked**
 [RRA08, SBI08]. **stacking** [CM09, DDBP09, HWTL03, KKY01, WRP⁺06].
standard
 [ASDP⁺06, CG06, FBDG06, KOFF09, LFSB03a, LFSB03b, SSS⁺09, SL04].
standing [KDG⁺09]. **staphylococcal** [JS07a]. **Starting**
 [VZVG06, BWI⁺02]. **state** [Ang09, BBI⁺09, CWY09, CFS⁺08, CHA⁺07,
 Chu07, CAG07, CMA⁺08, HM01, HNWF07, HNWF12, Hir08, HP05, IME02,
 JHZ09, KT02, Kri09a, LMK01, LZ05a, LDL⁺09, NTH09, PO03, PSS⁺04,
 POJ01, Qua07, SPS08, Sen06, SRE08, TH02, TST⁺08, TY03, TKN⁺08,
 WCFH02, WHF08, ZH08, ZOJ⁺06]. **state-correlation** [SRE08].
state-specific [TST⁺08]. **states** [Ang09, ABBC01b, Bof01, Bou01, CWY09,
 CNN07, DHM⁺03, DF04, EL07, FCW06, FDSA00, HFS⁺07, HYR06, HZ09,
 IR03, KUB07, LS08a, LWX07, LB08, MW09, MLCD01, NBTN04a,
 NBTN04b, OSA06, OV03, PRSMV08, Qua01, SBI08, SMKM00, VW00,
 WLZ⁺07, XZ05, ZL05, ZL07, ZL09b, ZM03, dSVA⁺09, ABBC01a]. **static**
 [FR0D08, LDG02, Mar03, XWL⁺09]. **stationary** [SK09]. **Statistical**
 [HFS03, PYEA03, DW08, EC06, Kob03, ML00, RK05, SBJ08].
statistical-thermodynamic [RK05]. **step** [BYQS03, BCP03, DLW06,
 KM00, KH06, MK02, Mck07b, OV03, Oos09, ZWZ09]. **step/particle**
 [BYQS03]. **stepwise** [LLKC06, LFS⁺07, NSB08]. **Stereodynamics**
 [CMLS05]. **Stereoelectronic** [DD08, PBF09]. **stereoisomers** [PCMG09].
stereoselective [AGI⁺00, AGI⁺07]. **Stereospecific** [PF06]. **Steric**
 [PBF09, BDW00, XYN⁺06]. **steroids** [AGMPRG⁺08]. **sterols** [CSU05].
STFs [DBS08]. **stiff** [ECA06]. **stilbene** [CJK⁺02]. **STO**
 [CGB03, RLRE01, RLER05]. **Stochastic** [Agr03, Fau01, KEM08, Sau04,
 AM09, CSJ01, DHF⁺05, GdSuM⁺07, MKT04, ZZ08]. **Stoner** [SK08]. **stool**
 [FKŠ⁺09]. **storage** [FR06]. **stored** [AT02, MBWP03]. **stored-integral**

[MBWP03]. **Strain** [ST01]. **strained** [ST01]. **strand** [GAS04, JS07b]. **stranded** [AZM03]. **Strategies** [DBS08, LJS05, YL09, EKB02a, EKB02b, KEB04, Vis02]. **strategy** [BME05, CZA03, LLL⁺08, MCF07, RI08, SMGE08, Wan09, WS02a]. **streamlining** [VGB08]. **strength** [DMJV05, FO08, SEKS09]. **strengths** [RM07]. **stretch** [Kle03, SDCG02]. **stretching** [CPDZH08]. **strictly** [FMSA06, TT01, TT05]. **Strike** [Ano06c, WZW⁺06]. **string** [Qua04, Qua07]. **strong** [LC07, PGG06]. **strongest** [VHRR07b]. **strongly** [ONHN00]. **strontium** [RD06]. **Structural** [CZFH07, EM03a, Kri09b, LWLS07, LFR07, MS03, BCP03, CKR08, CLF⁺09, ECM⁺03, GZ07, HYA02, HHP04, KZY09, Kar06, KPZK06, LL07, LJS05, NAT07, OFIK09, PK04, QLHL09, SLC⁺09, SVV⁺08, SRB06, XSHC06, XLC08, ZLJS03, ZWP08, CA07b]. **structurally** [AGMPRG⁺08]. **Structure** [BMTSC01, CDL06, HHWG08, HRR05, HS07b, ITS05, KCL06, KPR04, MN02, PGC05, PLC08, PHRR08, RG08, SG07a, AJ03, AGSFA⁺05, BED02, BS01, BAH⁺02, BAA⁺07, CLC03, CZB07, CDGS09, CDS09, CMaGL⁺04, CJS⁺03, CN05, CLA⁺00, CPUGD09, CSV⁺07, DP03, DHW⁺08, DHW⁺09, Fau01, FL07, FLOD07, FCP⁺04a, FL08, FLK⁺07, GBL⁺05, GTC06, GGGLL05, GdAcV⁺07, HHJ03, HEP⁺02, HN02, HP05, ILKR09, JCA⁺02, JLHF03, KP05, KFNH08, KHY00, KOFF09, KBK⁺01, KBL08, KIFK07, KWK⁺00, KGD06, LEK07, LJKL08, Lee09, LPP06, LZA02, LZ05a, LCSZ09, LW06, LOL⁺08, LYZ⁺08, LDL⁺09, LR03b, Loe03, LLL07, MOP⁺07, MM00, MLL08a, MM02, NK01, NYH02, NCO⁺05, OS08, PDP02, PSCD⁺09, PJB⁺07, PMM05, PRJ02, PF06, QB05, RPNJ07, RI07, RS05, RRS07, SSB⁺03, SJJ⁺04, SB01, SCP08, TD08, TT01]. **structure** [TGD05, Van02a, VHRR07b, WZY04, WMRW⁺01, WD08, WS07, XZZ04, YXL⁺09, ZZY07, ZZS⁺07, ZZY08, ZLD09, ZX08, vDSSvA04, vEMK01, vE01, RRCA08]. **Structure-based** [BMTSC01, HS07b, KBK⁺01]. **Structure-breaking** [HRR05, VHRR07b]. **structure-properties** [CDGS09, CDS09]. **structure-property** [JLHF03, PSCD⁺09]. **structured** [DC02]. **Structures** [AB00, CTFC08, HXD08, KS05a, PCMG09, RSSKB03, Ama02a, BK08, BSP06a, BS05, BRV⁺07, CUSS03, CWWS07, CRSB03, DW08, DF04, DSB⁺02, DB02, DJB02, EBAN07, FOL⁺04, GYCZ04, GJL⁺08, GCCVB00, HM01, HZ09, Hua09a, Hua09b, IGNH03, Kar01, KAS⁺07, KKMMMS04, LD05a, LWK08, LV08, LLXS02, LhWX07, LS05a, MKGA06, Mas01b, MHT01, PYCD03, PYS05, RI08, RSER09, RM00, RRS09, SO07, SHBD05, SWR06, TZX01b, TZX01a, TT08, TD06, VVBV02, WS05a, WB04a, WB04b, WB05, WDXS06, WS02b, WS07, Wu06, WWS07, WM01, XFF06, XLZ08, YIN03, YNW05, ZCL09, ZXY03, ZGXX06, ACM⁺06, FZL07, STC⁺08, UM03, ZXL⁺04, ZX09]. **studied** [AGO⁺02, CFC⁺08, DPT03, HFS⁺07, KBL08, LML⁺00, RGP⁺07, RJLR06, Sen06, SRE08]. **Studies** [JW12, ZWS⁺02, AB00, ADM⁺06, Ano06a, BY06, BPC01, BI06, BSJ01, BMTFR08, CMBC08, DBS07, EBAN07, FJ08, GYCZ04, GC04, GJK00, Han01, HSWW00, mJZyL⁺08, KCL06, KWK⁺01, KWK⁺02, Kle02, KZW⁺05, LYK⁺04, LWLS07, LDY⁺08, LJZ⁺07, LF02,

LWY⁺09, LSY02, MCR08, MK02, MOP⁺07, MW00, RPNJ07, RZWS07, SGPS09, SS00, SWBM08, SJJ⁺04, SLL⁺04a, SLHW09, SFR07, ST06, TJM⁺03, TMBM02, TCMS03, VS02, VMA03, VL00, VS08, WLL01, WLLS04, WLL07a, WyLG⁺09, WLL⁺03, WXX03, WCL05, WZXY07, WXK08, XLL⁺02, XKKL03, YIN03, YFR05, YLWL09, YLL⁺09, YKK09, ZDS⁺05, ZWL⁺05, ZZZ⁺06, ZAT07, ZXY03, ZL05]. **studio** [Gan09]. **Studd** [Ano06a]. **Study** [LSAS01, ŠBL05, YZ06, ZCS04, ABYM08, ASDP⁺06, Ama02a, Ama02b, ATH⁺03, AVB00, AZM03, BAL⁺01, BTP09, BSB09, BISB02, BL06, BLO⁺02, BRLS08, BRLS12, Bor03, BBSS06, BGC⁺09, BBI⁺09, BZL05, CMLS05, CC07, CFS⁺08, CUS00, CU01, CUSS03, CJS⁺03, CLFA07, CZFH07, CCCJ09, CJW⁺09, Che01, CN05, CNN07, CSB08, CFD03, CFD04, CPUGD09, ČJPZS08, CMD⁺04, CG05, CSB⁺03, DHM⁺03, DGD⁺05, DLR⁺08, DWS⁺09, Der09, DMC05, EA08, EBL⁺08, FÁ01a, FL07, FC06, FD03, FO08, FKU⁺05, FKM⁺06, FKM⁺07, FKŠ⁺09, GXK09, GHLK⁺02, GD09, Gog08, GM01, GLRL02, GGGLL05, GD06, GKTS04, GBBH09, HWFN01, HLLS05, HSF08, HELM09, HSMT04, HM08, HPL03, HK07, HJCP01, HHP04, HLMR06, IB04, IV04, IvSV06, IIK09, mJLzLyL07, JHZ09, JW00, JFG04, Kan07, KWHH07, KFD06, KSN01, KIFK07]. **study** [KS01b, KKMMMS04, KS05c, LD05a, LMK01, LKJ⁺04, LPK07, LWK08, LMCD09, Lee09, LZA02, LL01, LZJ03, LW04a, LX07, LWX07, LLL⁺08, LS02, LLS03, LMMW04, LS08b, LLKC06, LLW02, LKT04, LDT⁺02a, LDT⁺02b, LB08, LYZ⁺08, LDL⁺09, LMRVFH⁺09, LLL07, MWL⁺08, MGMM07a, MML⁺06, Mas01a, Mas01b, MDA08, McD03, McD08, MH09, MSBS01, MGG06, MH08a, MM02, ML00, MDI04, NTH00, NBTN04a, NBTN04b, NAT07, OO04, OON01, OY01, OY03, OSA06, OS08, OO08, Pac06, PP08a, Pan07, PNGG03, PGRRNG03, PC00, PFR04b, PG04, PHKG07, Pim03, PMPGP05, PMC⁺08, PRSMM03, PA05, PAS07, PMM05, PMM06, PWFS01, PHRR08, PB05, wQZsLyZ02, QtDg⁺08, RG02, RAGLL09a, RAGLL09b, RB01, RRS06, RP04, RD00, RGG08, RUPH06, RR05, SF07, SOOF05, SURG06, SBJ08, SG07a, SLL⁺04b, SMKM00, SBG09b, SN06, SPT⁺03, SCG04]. **study** [SE08, SSW⁺07, SK05, SLRC01, SVV⁺08, SMV⁺09, SSBE06, TBG00, gThDjL⁺01, TD08, TT02, UNHYT06, UNM⁺01, UM03, VHRR07b, WZY04, WC09, WMRW⁺01, WD04, WLX⁺05, WLLS05, WDS06, WDXS06, WDZS07, WLL⁺07b, WCW08, WWT08, WZZ⁺09, WM04, WOC⁺03, WD08, Won09, WDX⁺02, WRBV03, WC08, WJX⁺08, XYN⁺06, XB08, XDS06a, XFF06, XWXC08, XKG⁺05, XPW09, YT03, YT04, YTY07, YXZ⁺04, YDWS06, YXC⁺07, YLZ08, YLW⁺08, YQQH09, YHD⁺06, ZP03, ZPL07, ZZL04, ZLLS04b, ZLLS04a, ZLLS05, ZLLS06a, ZLLS06b, ZZW⁺07, ZZL⁺08, ZZL⁺09, ZH08, ZWY⁺09, ZOJ⁺06, ZNLL07, ZX08, ZTP⁺08, ZL07, dSVA⁺09, dRLMS00, NBJ04]. **studying** [AGI⁺00, AGI⁺07, dVB01]. **styrene** [Ama02a, Ama02b, XPW09]. **subspace** [FS00b, Har04]. **substance** [CCP04]. **substances** [ATH⁺03]. **substantially** [RK05]. **Substituent** [JWB05, Lee09, PWFS01, BPC01, HMMS09]. **substituents** [PSF⁺08]. **substituted**

[AVB00, BE06, BE07, HM08, HWGB01, LST08, MMMY07, MRS09, OSA06, PB05, RP09, TTB01b, WyLG⁺09, WW04, YDWS06, WFHP01].
Substitution [ZZS⁺07, BSB05, JT06, LFBSK07, SOOF05, SSB07, ZWS⁺02].
substitutional [FSS00]. **substitutions** [CM09]. **substrate** [BMTFR08, LCC09]. **subtype** [FTLV01]. **subunit** [OON01]. **subunits** [MML⁺06, PHFC04]. **successful** [CLA⁺00]. **successful** [IR03].
successively [YK08]. **suffice** [LLW⁺09]. **Sugiura** [TKN⁺08]. **suitability** [FMSA06]. **suitable** [GL04a]. **sulfate** [ZZW09]. **sulfation** [CLS⁺09]. **sulfide** [DLR⁺08, GGGLL05]. **sulfonylurea** [XYN⁺06]. **sulfoxide** [CFD04, EBDPM00]. **sulfur** [BT00, CGB⁺09, SO09, SW06, TTB01a, WS05b, FNP⁺06]. **sulfuryl** [CQ04].
sum [Bou01, SG01, UKN04]. **sum-over-states** [Bou01]. **summation** [Ami00, San01, SG01]. **sums** [KF02b]. **super** [RP07a]. **superatoms** [LWW⁺06]. **supercell** [EL09]. **supercells** [MOP⁺07]. **supercomputers** [VSK⁺04]. **superconducting** [MDI04]. **supercritical** [HTN03].
superexchange [WL00]. **superimposition** [ZA07]. **Superlinear** [FR06].
supermolecule [BA03, BA04a, vDSSvA04]. **superoxide** [PMM06, RJLR06].
superposition [COS01, CSD05, GRCD01, GCD04, IO08, Mas04, VKP⁺08, VZVG06].
supershort [XWL⁺09]. **Support** [CLXC02, LJZ⁺07, YMT04, CLS⁺09, HL08, LCC09, QLHL09, Mui05].
supported [GTC06, KEM08, SD09]. **suppressants** [LDC⁺07].
supramolecular [AM07, CMàGL⁺04, Won09]. **surface** [ABBC01a, ABBC01b, BMLV04, BL05, Bof01, BHH⁺09, CF06, DLD⁺02, DR09, EBL⁺08, GZL02, GCD⁺08, GB04, HHS⁺05, HG08, JBGK08, KLH⁺04, KCK⁺08, Lab08, LMK01, LFBSK07, LJ04, 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-adsorbed** [DR09]. **surface-doping** [JBGK08]. **surface-generalized** [YJF06]. **surfaces** [ATH⁺03, BHW00, BWZ08, DLD⁺02, EKB02a, EKB02b, ENM⁺04, FKJ⁺01, GSB09, HSF08, HHP04, IC08, IDMC09, JB04, KEB04, MCF05, MS00, PBZ00, Rap06, RKA⁺09, SPDS01, Sch03, Sha02, SBG09b, ST04, YJF06, ZBS03].
surrogate [Mck07a]. **surrounding** [KGL07, Yos02]. **survey** [HS07a]. **SuSi** [CA04]. **SVD** [CSD05, WG02]. **SVMTM** [YMT04]. **swarm** [CZB07, LJZ⁺07, SJJ⁺04, CLH⁺07]. **switch** [SF07]. **switching** [GG09].
symmetric [AT02]. **symmetrically** [Lai07]. **Symmetry** [PDC⁺08, PCA⁺08, BB08, CAGR08, FCP⁺04b, LWX07, SZW⁺05, WLPF05, Ell07, PV03, PTC01]. **symmetry-adapted** [FCP⁺04b]. **Symmetry-driven** [PV03]. **Symmetry-generation** [Ell07]. **Synergistic** [GS08]. **syngas** [YQQH09]. **synthase** [BBSS06]. **synthesis** [HLC09, PHR⁺05, WLL01].
synthetic [NHH05, WG02]. **system** [BL00, HELM09, HRBKB03, IS03, KYL03, LHJ⁺06, LCGA03, LDTS07, MM03, PGH⁺04, PRSMM03, Rud05a, YOB⁺08, ZAT07]. **Systematic**

[AST06, CS03, KWHH07, Kob03, LSAS01, MV06, PK04, PG04, RS05, WM04, WZXY07, ZXY08, Dya02, PWFS01, PV07, SYY⁺03, WK01, EA06, LMH⁺09]. **systems** [AS00, BHW00, BP01, BME05, BGJ01a, BWI⁺02, CN03, CG06, CvG08, CCK01, CMGDAC⁺07, DXW08, DRMD03, Don08, DK01, EGSG00, Ell07, FZL07, Fau01, GLMV09, HT03, JCA⁺02, JTR05, JG03, KSS08, KKC05, KAK⁺09, KBL08, Kle02, Kle03, Kri09a, LMJ02, LC09, LLL03, LDG02, MMLC05, MKGA06, MTB09, MM07, MS01, Oos09, RLDI09, RSN⁺02, Rud05b, Rud05c, SRS07, SS00, SYY⁺03, SWV⁺05, ST01, TH02, TT08, WWL⁺09, WNH03, YCXY03, YZ04, vdVGDM00].

T [BBI⁺09, Lu09, PFJ⁺03, ZKZ⁺07, DLD⁺02, Ike04, KVS⁺06]. **T-cell** [KVS⁺06]. **table** [Kau07, Nil09, SRB06]. **tableaux** [SN00]. **tables** [ARL01]. **tabu** [MGJAARC00, SE07, SE08]. **tailoring** [BG03, KKG⁺09]. **taking** [SN06]. **TaN** [ZHMW09]. **tandem** [UNHYT06]. **tantalum** [Tie09]. **target** [FM00]. **tautomeric** [LS08b]. **tautomerism** [YXZ⁺04]. **tautomerization** [BA03, BA04a, BA04b]. **tautomers** [HHWG08, PG04]. **TCNE** [GYMN07, TD08]. **tCONCOORD** [SD09]. **tCONCOORD-GUI** [SD09]. **TD** [CHA⁺07, SBI08]. **TD-DFT** [CHA⁺07, SBI08]. **TDDFT** [SL04]. **TDHF** [QCK01, QCK02]. **Te** [HKHN08, WWS07, HWFN01]. **technique** [COS01, GKH05, KLM⁺09, SATO04, TS05]. **Techniques** [Woo01, You11, AM06b, DC02, FSM09, KH05, PAT⁺09, PDS01, VE09, WSM⁺09, vGGB00]. **Teller** [Kri08, VDM06]. **temperature** [FGR07, JS07a, KT02, KGD06, MN02, TD08, XK08]. **temperatures** [KK01b, TK08, WHH⁺06]. **tempered** [BBP09, CVVB04]. **tempering** [SPT07]. **templated** [ST04]. **tensor** [BZP09, BAÅ07, RI07]. **tensors** [CDL06, KRM⁺02, ZLD09]. **term** [JČHS07, 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, SBI08, SM03]. **Testing** [CMàGL⁺04, BG03, PZS04, WWC⁺04, WWC⁺05]. **tests** [KSB⁺02, NGTB03]. **tetraammonium** [CW02]. **tetraazanaphthalenes** [CdML06]. **tetrachloride** [DMN05]. **tetracoordinate** [MMRVH07, SRS07, Wan09]. **tetracyanoethylene** [LH02]. **tetracyanoethylene-contained** [LH02]. **tetracycline** [AS06, AS09]. **tetrads** [MHS05]. **tetrahedral** [LSY02, OBT09]. **tetrahydroimidazo** [SPGS08]. **tetrahydroimidazo-** [SPGS08]. **tetrahydroouranylate** [IvSV06]. **tetramer** [RCA08]. **Tetraoxide** [JW12, SLHW09]. **tetrapeptide** [DSR⁺07]. **tetrapeptides** [GKTS04]. **Tetrazine** [JW12, SLHW09, XZ04]. **Tetrazino** [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, DVRP⁺03, FL08, GCD⁺08,

JHMB⁺⁰⁹, JHMB⁺¹¹, Lee09, Owe05, PCMG09, SWM04, SRK⁺⁰⁰, WWT08, YLWL09, ZXL⁺⁰⁴, ZWY⁺⁰⁹. **them** [YNW05]. **theorem** [Kar01, RLER07]. **theoretic** [SWZS04]. **Theoretical** [Ano06a, AZM03, BY06, BI06, Bor03, BS03, CNN07, CFD03, CFD04, CG08, COMR⁺⁰⁴, FJ08, FL07, FDSA00, GYCZ04, GLH⁺⁰⁸, HLLS05, HS00, IGL07, IIK09, mJIZyL⁺⁰⁸, JW12, KYFW07, KZY09, KSN01, KS05c, LS08a, LH02, LWX07, LDY⁺⁰⁸, LLW02, LDT^{+02a}, LDT^{+02b}, LYZ⁺⁰⁸, LMRVFH⁺⁰⁹, MMLC05, MCK05, MBM⁺⁰⁰, NBTN04b, OCP02, OKE⁺⁰², PFR04b, wQZsLyZ02, RTG00, RZWS07, SLL^{+04b}, SFR07, ST06, TKS⁺⁰¹, TJM⁺⁰³, gThDjL⁺⁰¹, VS08, WLL01, WLLS05, WDS06, WDXS06, WDZS07, WLL^{+07b}, WCL05, WJX⁺⁰⁸, XFF06, XKKL03, YTY07, YIN03, YFR05, YLW⁺⁰⁸, YQQH09, YLWL09, YHD⁺⁰⁶, ZLLS04b, ZLLS04a, ZLLS05, ZLLS06a, ZLLS06b, ZZW⁺⁰⁷, ZZL⁺⁰⁸, ZZL⁺⁰⁹, ZZW09, ZXY03, ZL07, BGC⁺⁰⁹, CN05, DLR⁺⁰⁸, GXK09, Ham07, HRBKB03, HLMR06, Kan07, KKMMMS04, LC07, LD05a, Lee09, LL01, LLKC06, LB08, MM02, MDI04, NTH00, NSB08, Nye07, OON01, PGRRNG03, PC00, PAS07]. **theoretical** [RAGLL09a, RAGLL09b, RRS06, RP04, RJLR06, SLHW09, SMV⁺⁰⁹, UNHYT06, WLZ⁺⁰⁷, WSM⁺⁰⁸, Wou00, XWXC08, YXZ⁺⁰⁴, ZL05, dRLMS00, Li01, NBTN04a, RD00, UNM⁺⁰¹, ZPL07, ZLD09]. **theoretically** [WS02b]. **theories** [JHZ09]. **Theory** [BBC⁺⁰⁵, SH08, WM12, ALTB06, ASDP⁺⁰⁶, ASY01, BC06, CWY09, CFK08, CR08, Chu07, CKW09, CPML08a, Cul08, CGSdST06, DPM09, DSR⁺⁰⁷, Ell07, EKB02a, FCW06, FZL07, FG02, FII⁺⁰⁷, FLGW00, FS04, FLK⁺⁰⁷, FZL⁺⁰⁶, GM01, Gri03, Gri04, Haf08, HSMT04, HS07a, Ho105, ION07, IKN08, IN08, JČHS07, KSS08, KWK⁺⁰¹, KWK⁺⁰², KK08c, KZW⁺⁰⁵, Kut07, LMB08, LF04, LFZS04, LMGR05, LF02, LLZL09, LDL⁺⁰⁹, Lu09, MGMM07a, Mat03, MW09, MA09, MH08b, ML00, NYH02, NUH02, NTH09, OFIK09, OKE⁺⁰², PFJ⁺⁰³, PSF⁺⁰⁸, PU09, PA05, QTdG⁺⁰⁸, RB01, RDM⁺⁰⁸, RZWS07, SH07, SH02, SZT08, SSMW09, SSB07, SW06, TST⁺⁰⁸, Tru07, TKN⁺⁰⁸, TKH03, WRP⁺⁰⁶, WB07, WZY04, WMRW⁺⁰¹, WW03, WCHW09, WL00, WCFH02, WNH03, WCL05, XYN⁺⁰⁶, XB08, XL02, XPW09, YCXY03, YH09, YYW07, YLL⁺⁰⁹, ZZL04, ZH08, Zho06]. **theory** [ZFL⁺⁰⁵, dOMSL01, vGGB00, vLBBR12, Blo04, BE09, CGMPT⁺⁰⁸, GGB07a, PFB05, PMC⁺⁰⁸, SG07b, ZSC05, Bic09]. **theory-based** [XL02]. **Theozyme** [UTH⁺⁰³]. **there** [KT02]. **thermal** [LZZC09, LLKC06, Lu09, SFRS01, WXK08]. **Thermally** [ZALMG03]. **Thermochemical** [BT00]. **thermochemistry** [LLXS02, ZXL⁺⁰⁴]. **Thermodynamic** [NA06, WR07, WFR08, ZWP08, Blo04, BZL05, KS05b, KK01b, LC06, LLZL09, RK05, SY09]. **thermodynamical** [KZY09]. **Thermodynamics** [UNM⁺⁰¹, HFSD03, JMD⁺⁰², MH09, NSU⁺⁰², PCMG09]. **thermoelectric** [XK08]. **thermostats** [MZL08]. **these** [LL00]. **thiamin** [LS08b]. **thiazoline** [XKG⁺⁰⁵]. **thio** [MMMY07, TTB01b]. **thio-substituted** [MMMY07, TTB01b]. **thioacetalization** [RUPH06]. **thioamide** [LKJ⁺⁰⁴].

thioamide-containing [LKJ⁺04]. **thioether** [SFR07]. **thiolate** [DMN05, SGD06]. **thiomandelate** [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, BP01, Bie04a, BB08, 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]. **tilt** [LHI09]. **TIM** [AGK03, LD05a]. **Time** [Bac09, CP08, Gog08, Kol04, LDL⁺09, Whe08, ZH08, BYQS03, CFK08, CPC⁺00, DF06, FCW06, HNWF07, HNWF12, HS01, ION07, KMH02, KM00, KH06, MW09, NTH09, PK05, PSF⁺08, TYN05, TST⁺08, TKN⁺08, YH07, ZWZ09, ZM03, vGGB00]. **Time-averaged** [CP08]. **Time-dependent** [Bac09, Gog08, LDL⁺09, Whe08, ZH08, CFK08, FCW06, HNWF07, HNWF12, HS01, ION07, MW09, NTH09, PSF⁺08, TST⁺08, TKN⁺08, YH07, ZM03, vGGB00]. **time-frequency** [DF06]. **Time-reversible** [Kol04]. **time-step** [KM00]. **times** [DDVD09]. **timescale** [MST⁺08]. **TiN** [JD09]. **TINKERTM** [Sto05]. **TiO** [FHRR07]. **TIP4P** [HPL03, THHN01]. **tires** [LMGR06]. **titanium** [UNM⁺01]. **Tl** [VHRR07b, VHRR07a]. **TIN** [ZX08]. **TIX** [ZL09b]. **tm** [BM00, GM01]. **TMPyP** [AZM03]. **toluene** [GCCVB00]. **tomography** [RGG08]. **tool** [ALB09, ÁCD⁺03, CCL06, CA07b, Gra07, HHG⁺09, LAEL01, LOL⁺08, NSU⁺02, OML⁺00, Pra01]. **toolkit** [Hin00]. **tools** [MRS09, Nye07]. **topo** [GRCD01, GCD04]. **topo-geometrical** [GRCD01, GCD04]. **topological** [CAGR08, DRAS04, DRAS05, FSS00, GDPCPU07, HM08, JLHF03, MP03a, RP07c, RP07b, SFC04, YWHZ03, ZSE08, ZNLL07]. **Topology** [RSER09, FCP⁺05, GdAcV⁺07, Kle03, KF03, KBL08]. **Topology-based** [RSER09]. **Tork** [CG03]. **torsion** [Ano06c, CIB05, FWH⁺07, FKZ09, MGLDS00, OMNH08, PHR⁺05, TNS00, WZW⁺06]. **Torsional** [PSF⁺08, DHF⁺05, FPG⁺06]. **torsions** [SP05]. **total** [RP07a]. **toxicity** [CMCB08]. **Tp** [HT05]. **TpMXO** [HT05]. **trace** [KLS02]. **tracing** [Kli01]. **tracking** [HNR08]. **training** [AG03, LJZ⁺07, LSY02, SJJ⁺04]. **trajectories** [Ham07, MST⁺08]. **trajectory** [Qua07]. **trans** [BZL05, CSB08, HKHN08, KMM07]. **trans-** [BZL05]. **transamination** [LDY⁺08]. **transcriptase** [AJNG01]. **transfer**

[AGK03, BA03, BLN01, BL00, CXZ⁺09, CHRL09, FDSA00, FZL⁺06, GWM08, GVATG03, GGLR00, HFHL06, IN01, JJH01, LLM08, LMGO⁺09, Li01, LL01, LH02, LB05, LLS03, MT03, MAF⁺07, Mck07b, OON01, PGG06, PMPGP05, QZZZ03, Rao00a, SL09, TBG00, WL00, WC08, YS00, ZY01, ZH08, BA04a].

Transferability

[CSB⁺03, TT05, FDM00, KS01a, OSHS03, RSP03, TFZRG01]. **Transferable** [WBSR03, HXLS09]. **transferase** [SFR07]. **transferred** [GFS05]. **transfers** [XKG⁺05]. **Transform** [BWP07, HLM05, ON07, QLHL09, TYN05].

transform-based [HLM05]. **transformation** [PVdJB00].

transformational [CN03]. **transformations** [WSM⁺09]. **transformed**

[Nak02, NA06, vDSSvA04]. **Transition**

[FKRE08, LMGR06, TH02, ABYM08, ABBC01a, ABBC01b, Ano06a, Bac05, BP03, BS06, Bof01, BRV⁺07, BM00, BGJ01b, CWWS07, Chu07, DLW06, Dib05, EL07, GHH07, GM01, Hol05, JHZ09, KRM⁺02, LW07, LD05a, LH02, LGB⁺09, LWZ09, LK03, LK04, NR04, PYCD03, Qua01, Qua07, RRFC⁺03, SK09, SZT08, ST06, TKS⁺01, WB07, WL09b, YTH01, ZALMG03].

transition-metal [Ano06a, ST06]. **transitions**

[CZ05, FC06, JW06, OYK⁺09, SMK00]. **Translation** [RLER05].

transmembrane [GAS04, YMT04]. **transport**

[Ara04, CM09, FCP⁺04a, FCP⁺05, KK08c]. **treating** [MA09]. **treatment** [BCF⁺09, BZL05, CLA⁺00, CBH⁺03, HC08, HHH00, IB04, JB04, KS05b, KCL00, LS08c, MFB04, MR02, MGLL03, RI07, RP02, XL02]. **treatments** [CEP07, DWNB01]. **tree** [GY08]. **treecode** [DK01]. **Trends** [SRB06].

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

tribenzo [GLRL02]. **trichloroacetaldehyde** [CU01]. **tricoordinated**

[LTF⁺07]. **trigonal** [JHMB⁺09, JHMB⁺11]. **trimer** [LZJ03, RRCA08].

trimers [ABYM08, VS02]. **trimethylamine** [CPDZH08]. **trimethylsilyl** [LLKC06]. **triosephosphate** [AGK03]. **tripeptide** [VKP⁺08].

triphosphate [GS04]. **triple** [PP08a, RPNJ07]. **triple-decker** [RPNJ07].

triplet [CZ05, CG08, FDSA00, LS08a, OSA06]. **tripodal** [HA04].

trisaccharide [GBB07]. **tRNA** [GGT08]. **truncated** [KK08a]. **Truncation** [RRS09, MN02]. **Trypan** [SRK⁺00]. **Trypsin** [JZD⁺09, CWV⁺05, MBC08].

Trypsin-ligand [JZD⁺09]. **tryptophan** [HLC09, Li01, LL01, MM05]. **Tsi** [XFF06]. **TTTO** [JW12, SLHW09]. **tubular** [FL07]. **Tuczek** [Ano06a].

tumor [WCF04]. **tumor-specific** [WCF04]. **Tuning** [JHMB⁺09, JHMB⁺11].

tunneling [Chu07, MKT04, RWBH09, SFRS01]. **TURBOMOLE** [LLL03].

turns [HL08]. **Two**

[PFB05, Yas08, AMR04, AHK02, BRS07, BE09, CVR08, CCK01, DHF⁺05, FBDG06, FR06, GGP09, GYMN07, GGA00, HK08c, JJK⁺00, KAS⁺07, KT02, Lai07, LDC⁺07, LWW⁺06, Sen06, Sto05, Van02a, Van02b, YFR05, dSR08].

two- [Lai07]. **two-body** [FBDG06]. **two-center** [BRS07, GGA00].

two-component [Van02b]. **two-dimensional** [CVR08]. **Two-electron**

[PFB05, Yas08, FR06, GYMN07, GGA00, Lai07].

two-electron/four-centers [GYMN07]. **two-state** [KT02, Sen06]. **type**

[Bie04a, CXZ⁺09, CJK09, CVVB04, EdIVR⁺03, GC02, Gri06, HLC09, IKN08, KDG⁺09, Leh06, MY08a, OON01, SDL⁺09, TW03, TLOG00, VB03, WD08, YXC⁺07]. **types** [BY06, GGP09, KS05b, MLL⁺08b]. **Typical** [SMV⁺09, MLL⁺08b]. **tyrosine** [AG00, CLS⁺09, LRI⁺02, Li01, LL01, OO08].

U [Han01, CCCJ09, GHLK⁺02, RLDI09]. **ubiquinone** [IN01]. **ubiquitin** [KIFK07]. **UCSF** [PGH⁺04]. **UF** [Han01]. **UK** [Lip00]. **ulcerogenic** [CMBC08]. **ultra** [ZHMW09]. **ultra-incompressible** [ZHMW09]. **Ultrafast** [BR07]. **ultrasoft** [PSS⁺04, PSMB05]. **umbrella** [RNG03]. **unbiased** [Pul05, SYC08]. **uncertainty** [SY09]. **unconstrained** [DMN03]. **uncorrected** [PSC⁺01]. **understand** [DSB⁺02]. **Understanding** [CAGR08, CDPL09, BRS07, ZZW09, CFER04, HP04]. **Unicorns** [FK07b]. **Unified** [GDPP08, CMGDAC⁺07]. **uniform** [HdMdS05, HdS06, HD06, Rap06]. **Unimolecular** [ML00, FS00b, KZY09, ZZL04]. **unique** [KT02]. **unit** [VM07, Yas08]. **unitary** [KBT03]. **units** [CXZ⁺09, FEV⁺09, HP05, NK01, NL08, PC00, PFC03]. **Universal** [DHW⁺00, HdMdS05]. **Unorthodox** [KBB09]. **unphysical** [OV03]. **UNRES** [HXL09, NCO⁺05]. **unrestricted** [YH07]. **unsaturated** [BS03, KFD06, MTB09, Wan09, ZKZ⁺07]. **Unusual** [XK08]. **UO** [IV04, IvSV06, RDM⁺08]. **Update** [BKS02]. **updated** [Chu07]. **Updates** [Ano04b, BACJCT01, DvL01, Gly06, JVVK09]. **upon** [OFIK09]. **uracil** [LMGO⁺09, MSBS01, MHS05]. **uracil-base** [MHS05]. **uranyl** [IV04]. **Urea** [SK05, AS00, VVS07]. **ureases** [ESM06]. **Use** [BWI⁺02, DW08, Wou00, ALB09, FC06, JNV08, Kli01, MRC03, OCP02, PRKP05, PRS04, RCJ02a, RSN⁺02, Ruv07, SH07, SVT09, VGGMM05, YTH01, YZ04]. **used** [DvG00, ESP04, HdMdS05, HdS06, HD06]. **user** [DPDG05, JKII08]. **uses** [KBB09]. **Using** [CSD04, FSM09, HL08, Kne05, LL07, MO01, OSHS03, QLHL09, SWR06, XSHC06, XLC08, XOW⁺00, Adc04, AJ03, ABWT09, AM06b, AS00, BWP07, BMLV04, BVW04, BME05, BGC⁺09, Bud07, CLWL09, CN03, CSJ01, CLC09, CKR08, CLA⁺00, Chu07, CP08, CP09, CCP04, CPML08a, CGSdST06, DLD⁺02, DWNB01, DR09, DVP⁺02, DB06, DB02, DMJV05, EKO⁺01, EKB02a, EM03b, FCW06, FMPS08, FBDG06, FAB⁺00, FEVM01, FR06, FSFK05, GMA04, GL04b, GdSuM⁺07, GPSP06, GGLR00, Haf08, HWDB03, Han01, HSMT04, HSM06, HMMS09, HG08, HHP04, II02, IS07, IS03, IT03, IK00, JBGK08, JIK09, JVVK09, JTR05, JFG04, JSHG07, KRM⁺02, KKG⁺09, KM00, KLH⁺04, KK08c, KOFF09, Kle02, Kle03, KBT03, KKS04, Lab08, LCKL05, LCC09, LZ05a, LLL⁺08, LZZC09, LS05a, LZ05b, LSY02, LKW04, MWL⁺08, MT03, MMLC05, MKT04]. **using** [MV06, MBP09, MOP⁺07, MTE04, MRS09, MRS⁺07, NCO⁺05, NINAT⁺07, OFB08, OKE⁺02, PMB04, PS09a, PAT⁺09, PP08b, PDS01, PZS04, PSS⁺04, RI07, RI08, RMP01, RG08, RON02, SDL⁺09, SPGS08, SSB⁺03, Sch00, SRCD03, SBG⁺09a, SY09, SPT07, SMV⁺09, TP01a, Tie09, TCSM03,

UBDPJ04, VSW⁺⁰³, Van02a, WLZ⁺⁰⁷, WL00, WEE01, WG02, WOC⁺⁰³, WCS09, XLT07, YK00, YYW07, ZCS04, ZBS03, ZWP08, ZHH09, vdVGDM00, PRSMM02]. **utility** [KMH02]. **utilization** [GS08, DMLI05]. **utilizing** [NYTH09, Wan09].

v [Lip00, ZZW09, GBJ03, Kri09b, PFC03, TD08]. **vacancy** [ZMH⁺⁰⁹]. **vacuum** [BISB02]. **Valence** [LW07, SH08, Tru07, WM12, Bic09, BLT03, Cul08, EA08, HELM09, HS07a, May07, MG00, PRSMV08, SWZS04, SMZW05, SSMW09, SSW⁺⁰⁷, VBGL⁺⁰⁰, WMRW⁺⁰¹, WJ00, dSVA⁺⁰⁹, vLBBR12]. **valent** [AZM03, CN05, GWL07]. **Validation** [BAÅ07, VCM01, AGI⁺⁰⁰, DGD⁺⁰⁵, JJB02, JCL05, JVVK09, MSR04, MTE04, SRB06, APG05, HZ06b, NGTB03]. **valinamide** [HJCP01]. **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** [ŠBL05]. **various** [BP07, HMMS09, IT03, Kró03, KS01b, MLL^{+08b}, PP08a, PFJ⁺⁰³, PMM05, RR05, WHH⁺⁰⁶, ZCL09]. **varying** [CC09]. **VASP** [Haf08]. **VBSCF** [vLBBR12]. **VCH** [Sta00]. **VDD** [GHBB04, GHBB04]. **vector** [CLXC02, CLS⁺⁰⁹, HL08, LCC09, LJZ⁺⁰⁷, QLHL09, YMT04]. **vectorizing** [SO07]. **vectors** [BWI⁺⁰²]. **versatile** [KF08, TdMSD⁺⁰⁸]. **version** [HDBD04]. **versions** [Sto05]. **versus** [ABYM08, ALC08, BSG07, BB08, JS07b, JBGK08, LST08, LTV08, PSMB05, Van02b]. **Vertical** [PRSMM03, SA07, CG08, LWX07, LFEdL06, SLRC01, TKS⁺⁰¹]. **VI** [HP05]. **via** [BA03, BA04a, Bou01, BRS00, 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, ZWPR⁺⁰⁴]. **Vibrational** [BP07, CLP⁺⁰⁵, LC09, NR04, WB07, BRV⁺⁰⁷, DB07, GBDP05, Gra07, Han01, HNR08, JARM02, LMB08, LN01, MR02, NRKH02, NAT07, PZWG⁺⁰⁴, Tor02, WM04, WM01]. **vibrations** [CPDZH08, DR09, KCL00, vE01]. **vibronic** [TP01b]. **view** [CSJD04, Jac09, JMD⁺⁰², MGCA07]. **VIII** [EBD⁺⁰¹]. **vinyl** [YYW07]. **vinylphosphine** [MGLDS00]. **viridis** [IN01, OON01]. **virtual** [GFS05, KSM05, LZ05b, PRDS08, YOB⁺⁰⁸]. **virus** [AJNG01, DLRZ09, KCL06]. **viscosity** [ZP03]. **Visualization** [MMP⁺⁰⁷, RP07b, ARL01, KYL03, PGH⁺⁰⁴]. **Visually** [SD09]. **VMD** [Pra01]. **VMFCI** [CCL06]. **VO** [PV07]. **voltammetry** [KJP⁺⁰⁷]. **Volume** [Sta00, BVW04, Lab08, LFSB03a, LFSB03b, Mue01, QNF09]. **volume-preserving** [QNF09]. **volumes** [BHH⁺⁰⁹, Rao00b, SBLK01]. **Voronoi** [GHBB04, MVLG06, SBLK01]. **VP1** [KCL06]. **VPP700** [KSY⁺⁰⁰]. **Vpu** [KF08]. **vs** [CXZ⁺⁰⁹, LLKC06, MA05, SCG04, Wib04].

W [UM03, WWC⁺05, MH09]. **W2** [dOMSL01]. **Waals** [AD00, CPUGD09, GdSuM⁺07, Gri04, KLH⁺04, LS08c, VS02]. **walk** [CY09, CY13]. **walking** [BHG03]. **wall** [BG07]. **walled** [XWL⁺09, ZZvRSC08]. **Wang** [Ano06c, GHH07, JW12]. **warping** [JO02]. **Water** [LMIF06, Mor02, NK01, BLL⁺06, BUMCMRL00, BRLS08, BRLS12, BSH07, CCK01, CSB⁺03, DLR⁺08, DWS⁺09, DSB⁺02, ES00, FG03, FBDG06, FKŠ⁺09, GWM08, GDV03, Gol09, HM02, HRBKB03, HPL03, HFHL06, HN02, HTN03, HLMR06, ITS06, IDMC09, KFNH08, Kle02, Kle03, LPB03, MT03, MN02, MZ05, MG00, OCP02, PHJ⁺08, PPYS08, RR05, SO07, SSM08, SJW09, SVV⁺08, THHN01, Tot04, UM03, VHRR07a, VHRR07b, VL00, WL09a, WD04, WDWS06, XKG⁺05, YT03, YSJ09, Yos02, YGLvG06, ZX04, ZCZ03, ZZY07, ZZY08, ZWP08, BA04b, WJX⁺08]. **water-addition** [RR05]. **Water-assisted** [BA04b, WJX⁺08]. **water-phase** [KFNH08]. **WATGEN** [BSH07]. **Wave** [GBJ03, Bac04, Bac07, Bou00, GFS05, MLL06, PFB05, PSS⁺04, PSMB05, RLDI09, TT05, VSK⁺04, YH06, YLL⁺09]. **wavefunction** [IS07]. **wavefunctions** [BWW⁺08, KTM02, PJPJdPRMI07]. **Wavelet** [CF04, ON07, QLHL09]. **waves** [MOP⁺07]. **way** [GZ07, HSWW00, PRSMM02, VBGL⁺00]. **weak** [QTdG⁺08]. **weakly** [CPML08a, JRJ01]. **web** [KKG⁺09, GKRG08, Gra07, JKII08]. **Web-based** [Gra07, JKII08]. **web-interface** [KKG⁺09]. **WebMTA** [KKG⁺09]. **WebProp** [GKRG08]. **Wei** [Ano06c]. **weight** [AG00]. **weighted** [FS00b, HWDB03]. **weights** [Bac04, Bac05, Bac07, Kar01]. **Weinhold** [GHBB04]. **well** [BBP09, WCK00]. **well-tempered** [BBP09]. **where** [HYA02]. **which** [SBH02]. **Wiener** [YWH04]. **Wiley** [Bic09, Lip00, Sta00]. **Wiley-VCH** [Sta00]. **Will** [LLW⁺09]. **Windock** [HS07b]. **Windows** [HS07b]. **Windows-based** [HS07b]. **wise** [Nil09]. **within** [Der09, FDM00, GS09, KC01b, MY08b, NYTH09, NAT07, SHBD05, SPT⁺03]. **without** [AL01, HdMdS05, HdS06, HD06, HZ09, Nil09, PK05, Qua07, RKA⁺09, TW03]. **WNO** [HT05]. **worker** [FCK⁺08]. **worker-based** [FCK⁺08]. **Working** [Nye07]. **World** [Woo01, You11, FK07b]. **worlds** [Sim07]. **Wu** [Ano06c].

X [BAL⁺01, BPC01, CRC⁺08, Dib05, HZ09, Hua09a, KBL08, LS08a, Mck07a, Mck07b, OS08, RB01, STC⁺08, WLLS04, WZZ⁺09, WWS07, ZJM⁺07, ZY01, ZL09b, HYA02, HSWN01, HN02, Lip00, Mar03, Sta00, WKYU01]. **X-ray** [HSWN01, HN02, WKYU01]. **xanthate** [CFD03]. **XCu** [KBL08]. **xenobiotics** [PCMG09]. **xenon** [HdS06]. **XES** [EKO⁺01]. **Xiang** [Ano06c]. **Xinli** [JW12]. **XMVB** [SMZW05]. **XPS** [EKO⁺01]. **XX** [CRC⁺08]. **XXXIII** [JPF⁺00]. **XXXI** [HJCP01]. **XXXIII** [PFJ⁺03]. **XY** [ZY01]. **xylose** [GVATG03].

yield [CSD05]. **YL** [NYK⁺09]. **ylide** [LS08b]. **ylides** [Mit01]. **Ylidic** [XDS06b]. **yloxy** [BE07]. **Yong** [Ano06c]. **young** [SN00, Woo01]. **ytterbium** [FRS05].

Z [CRC⁺08, PWFS01]. **zeolites** [LTV08, SDCG02, TLOG00]. **zeolitic** [Tie09]. **Zerner** [Ano00]. **zero** [RKA⁺09]. **zero-flux** [RKA⁺09]. **zeta** [CMJ08]. **Zhang** [Ano06c]. **Zhi** [Ano06c]. **Zhi-Xiang** [Ano06c]. **Zinc** [CFS⁺08, BSDM04, ECM⁺03, JT06, JT08, KZRO03, RGP⁺07, SFR07, SCF⁺09, SDM02]. **zinc-**[SDM02]. **Zintl** [XB08, ALC08]. **zirconocene** [LHP01]. **Zn** [BTP09, GPSP06, BBI⁺09, ESM06, FO08, GPK05, ROG00, TGGP⁺00, TFZRG01]. **Zn-biomimetic** [FO08]. **ZnO** [HSF08]. **ZnX** [WWS07]. **Zori** [AGSFA⁺05]. **ZPE** [MGLDS00]. **ZPVA** [QCK01, QCK02]. **zwitterionic** [ROG00]. **zwitterions** [KLB03]. **zymogen** [PDP02]. **ZZ** [CRC⁺08].

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