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$(0.0 \leq x \leq 0.3)$ [WZ99]. (110) [Bre99, GL92]. $(4s)$ [KSW98]. $(5s)$ [KSW98]. (C_{2v}) [AFM99]. $(d+s)^3$ [Bec97a]. (Γ) [LMAK93]. $(n = 0, 1, 2)$ [WMZ98]. $(n = 1, 2, , 6)$ [HL93b]. $(n = 1, 2, 4)$ [XKB+99]. $(n = 1--4)$ [ST97]. $(n = 1--6)$ [GFY+99]. $(n = 13)$ [IBS95]. $(n = 2--4)$ [CCS99]. $(n = 2 - 14)$ [Bou94]. $(n = 2 - 4)$ [SPR94]. $(n = 2\text{to}6)$ [KSN93]. $(n = 4, 5, 6)$ [RT98]. $(PW_{12}O_{40})^{3-}$ [CJX+92]. $(SiH_3)_2F^+$ [Pal94]. $(x = 2--16)$ [LXWZ99]. + [BCY95, BYGA99, CR96b, MSM96, Oku98, SC95, XY95]. $1, 4$ [SWD+99]. $1 - x$ [GFRR94]. $1/r$ [Cza95]. $1/r_y$ [PCCO94]. $1/Z$ [GLMP98]. 12 [XSG97]. $1s\Sigma 2p\Sigma^1\Sigma_u^+$ [Brä68]. 2 [HGL99, SSM+99]. $2 + 2$ [Fir94]. 20 [LS99]. $2^1A_g^-$ [NNH98]. 3 [Boe91, Nag96b, RT99]. 4 [BT95, RT99]. $4n + 2$ [OS95]. 4×4 [Lin81]. 5 [MMCC99]. 540 [MUL99]. 6 [SSM+99]. 7 [SSM+99]. $< 1/r >$ [Csa94]. $< r^n >$ [Csa93]. = [Bou96a, BCY95, NBS95, PZTPMC99, STMR97, SG96a]. * [JKK+92, LJ95].

$^{+}$ [ANB94, BCMÖ97, BB95, CWZ98b, CLOFR98, Csa96, FV96, Gao93, HL79, JM93a, KKWT99, KGS93, KA95a, MMRSN92, NBS95, PS93, PHH94, Pro94, Pro95, SPS96b, SZ97b, STC96, TNSM99, WY99, WMD95, YD96, YSHD97]. $^{+(-)}$ [BCY95]. $^{+}_{2}$ [BK94b, ELMY96, SC95, ZTC97]. $^{+}_{3}$ [WSB94]. $^{-}$ [CLOFR98, Csa96, JPD67, KKWT99, KK93, KGS93, MTNF99, Oku98, Ort98a, SEKEB98, WYZ^{+}92]. $^{---}$ [Kal90]. $^{-}_{2}$ [ZTC97]. $^{-}_{I}$ [DM97b]. $^{-}_{II}$ [DM97b]. $^{-}_{II} \rightarrow$ [DM97b]. ^{0} [CBAM97]. ^{1} [BP93a, BYGA99, CBT93a, CRSP93, GAdAC97, HMK96a, HMK96c, HMK96b]. ^{119} [GAdAC97]. ^{13} [GS97b, GAdAC97, KH96a, RN96]. ^{131} [SCL96]. ^{17} [KH96a]. ^{19} [GAdAC97]. $^{1}A_1$ [CCS98]. $^{1}A\prime$ [KA96]. $^{1}B_u^{+}$ [NNH98]. $^{1}\mathrm{E}_{2g}^{-}$ [BČ95]. $^{1}\Sigma$ [CWJ^{+}99]. $^{1}\Sigma^{+}$ [BFV^{+}93, TGS99]. $^{1}\Sigma_g^{+}$ [BP93a]. $^{1}\Sigma_g^{+} - a^{1}\Delta_g$ [MLK94]. ^{2} [BKL97, BLK97, BP93a, ELMY96, Man99, PS93, Sel93, SZ97b, WY99]. $^{2+}$ [BL99, BB95, BDH^{+}97, CAJ95, CG97b, DWB98, EJ93, JM93a, KGS93, MMRSN92, OSS95, TJ97, Wil90]. $^{2+/3+}$ [ZBL99]. $^{2-}_{1}$ [LGT94]. $^{2-}_{4}$ [BADM97]. $^{2-}_{II}$ [DM97b]. ^{207} [GAdAC97]. ^{29} [GAdAC97]. $^{2}\Pi_g$ [MM94]. $^{2}\Sigma^{+}$ [LBG97]. ^{3} [BP93a, CBT93a, CRSP93]. $^{3+}$ [BDH^{+}97, DdJN95, MNC95]. $^{3-}$ [NG95]. ^{35} [GAdAC97]. $^{3}\Pi_g$ [TGS99]. $^{3}\Sigma^{-}$ [FV96]. ^{4} [HMLK98]. $^{4+}$ [ABCM93, SK99a]. $^{5+}$ [Cze99, SK99a]. ^{6} [Tew94, Tew97]. $^{6+}$ [SK99a]. $^{6-}$ [XYC98]. $^{7+}$ [SK99a]. $^{8+}_{4}$ [BB95]. ^{e} [BLK97]. $^{\infty}$ [KP97]. ^{M} [PAT93]. ^{N} [PAT93, KS95b]. $^{n+}$ [WMZ98]. ^{o} [BKL97]. $_{0.4}$ [Li97]. $_{0.6}$ [Li97]. $_{0.8}$ [Min96]. $_{1}$ [DM98, ELMY96, GJOV97, LGT94, MW92]. $_{1-x}$ [WZ99]. $_{1.2}$ [Min96]. $_{105}$ [RKPE95]. $_{111}$ [RKPE95]. $_{12}$ [Csa96, Eva97, TST^{+}99]. $_{123}$ [RKPE95]. $_{13}$ [LMC97a]. $^{2}_{1}$ [DM99]. $_{1A}$ [PW97]. $_{2}$ [AS93, ANB94, ACHT95, Ali99, ABCM93, ABDM94, ADM98, BA91, BILA95, BUZ94, BDNT97, BBC^{+}94, BP93b, BP93a, BHGC99, BML98, BB94, BYE^{+}97, BCY95, BDH^{+}97, CWX93, Cai93, Cai94, CPBC95, CR96b, CGG96, CB93b, CB94a, CF93, CPD^{+}98, CDP^{+}99, DSS90, DdJN95, DZ97, EBG95, FdCC92, FSBS^{+}95, FCVL98, FMD^{+}96, GKKM96, GJPZ97, Gin97, GS93, GJOV97, GZDZ97, GL96a, GL96b, HMGP93, HBL99, HP98, Hir92, IBS95, JMP99, JKK^{+}92, Jen94, JMD95, JJ97, Jur97e, KJ95, KA96, KP97, Li93, LF95, LV97, MSS95, Man95, MLT98, MHM95a, MECE97, MHY98, MK90, MLL99, MM94, MGNK95, MTD93, MTTS93, MCS98, MZ95, MDM94, MD91, NM95, NBS95, NL96b, OTS^{+}95, Oku98, Ort98b, PBS99, PSBL98, PPSK96, PPK97, PGS97, PK76, Pro94, RN96, RA91, RA97, RA96, RCWN94, RKH^{+}98]. $_{2}$ [Roz97, RP98b, RS97b, SE93b, SM96a, SCP^{+}95a, SAB^{+}97, SL93, SRP^{+}98, SX96, SZC97, SST93, STMR97, SCS94, SZCO99, SGGMGFS96, SES93, SG97, SGB98, Spe72a, Sta98b, SC95, STC96, SC99, SNH99, TJ97, TGS99, TMA97, TPR96, TFSZ95, TZCT97, TMD96a, TMD96c, VH96a, VJ95, VJ97, WY99, WI96a, WI96c, WI96b, WDS97, WL99, WMD95, YNMT98, YNST99, YD96, YSHD97, YK97, ZC96a, ZC96c, ZC96b, ZTC97, ZBL99, ZGPS97, vBN95]. $_{2}(A)$ [GL96c]. $_{20}$ [CXFP99]. $_{24}$ [WYW96]. $_{240}$ [CXFP99]. $_{26}$ [RG99]. $_{28}$ [LSC98]. $^{+}_{2}$ [Ata97a, BSHP97, CGG96, GSSD^{+}96, JEB92, LA97, LBG97, MUMH97, Pro95, RS97b, Sch97, SBOB97]. $^{-}_{2}$ [BMG95, CGG96, LBG97]. $_{2h}$

[BBC92]. $_{2n}$ [GFY^{+}99]. $_{2} \rightarrow$ [XFF98]. $_{3}$ [AMC97, BUZ94, Boe91, BDD93, CCC^{+}95a, CLOFR98, CEM^{+}96, DZ97, DM98, DLF99, FCVL98, Fra99, Gao93, GWB97, GAdAC97, Hag99a, JMP99, Jen94, KP96, Kal90, KJ95, KLO^{+}98, KGS93, LJ95, LDGA96, Li93, LF95, MCL95, MLT98, MGNK95, Moc99, Nag96a, Nag96c, Nag96b, Oku98, PZTPMC99, PCF94, PPSK96, PPK97, RN96, RA91, SL93, SRP^{+}98, SBAD90, SP91, SZC97, SL97, SC99, VX99, WY99, WL99, WMZ98, WZ99, XFF98, YK97]. $_{3-\delta}$ [Li97]. $_{3-y}$ [Min98]. $_{32}$ [XYC98]. $^{+}_{3}$ [BMG95, Hag99a, KLT97, TMA97]. $^{-}_{3}$ [NG96]. $^{2}_{3}$ [DM99]. $_{3}\cdots$ [PZTPMC99]. $_{3} \rightarrow$ [YD96]. $_{4}$ [AS93, ABCM93, BL99, BILA95, BUZ94, BHGC99, BBC92, BB97a, BL98, DZ97, FCVL98, GS93, Gut99b, HP98, JKK^{+}92, JKJ94, JG95, Jen94, KP96, KGS93, KC97, LSC98, LCS98, MVS97, MHM95b, MNC95, PCF94, RKG96, SC99, WYW96, WY99, WI96a, WI96c, WI96b, vBN95]. $_{40}$ [LCS98]. $^{+1}_{4}$ [MVS97]. $^{2-}_{4}$ [CCWCF96]. $_{42}$ [BBC92]. $_{4} \rightarrow$ [YSHD97]. $_{5}$ [CCC^{+}95a, DWB98, KJ95, KGS93, NM95, NG95, NG96, OSS95, RA91, SG96a, SG96c, SG96b, SC98b, SC99]. $_{5+\delta}$ [Min96]. $_{6}$ [BL99, BUZ94, BBC92, Bou96a, Bou96c, Bou96b, BDH^{+}97, Csa96, Cze99, DN96, DdJN95, JKK^{+}92, MLL99, RA91, RKG96, Spe72a, TJ97, Thu69, WG94, ZBL99]. $_{60}$ [BBZ91, BSS^{+}97b, CCC^{+}95a, DM98, DM99, HRRBL97, HL93b, LL99, SZCO99, TST^{+}99, TFSZ95, XY95, YZX96a, YZX96c]. $^{2-}_{60}$ [HOF^{+}97]. $^{3-}_{60}$ [HOF^{+}97]. $_{7}$ [Li93, SG97, WL99]. $_{70}$ [BBZ91, LFS94, TZCT97]. $_{78}$ [AS99, RG99]. $_{8}$ [BUZ94, CG97b, Csa96, Eva97, GSSD^{+}96, JG95, RA91]. $_{80}$ [CXFP99, SLA97]. $_{81}$ [REL^{+}90]. $_{86}$ [SLA97]. $_{87}$ [REL^{+}90]. $_{88}$ [SLA97]. $_{9}$ [KP97, XYC98]. $_{93}$ [RKPE95]. $_{B}$ [CMSF93]. $_{c}$ [DMB97, Fri93a, Fri93b, Li93]. $_{I}$ [DM97b]. $_{II} \rightarrow$ [DM97b]. $_{\infty}$ [FMD^{+}96]. $_{J}$ [Man99]. $_{n}$ [AS93, BDD93, Cas97, CCS99, GFY^{+}99, Ike99, IP93, IBS95, Kar90, LDP93, LCP^{+}91, MKRW99, NYKY98, ST97, SPR94, WMD95, XKB^{+}99]. $^{-}_{n}$ [KSN93]. $_{s}[\rho]$ [LBPL97]. $_{X}$ [YZX96c, BSS^{+}97b, GFRR94, LXWZ99, SZCO99, SL97, WZ99]. $_{x}[\rho]$ [LBPL97]. $_{y}$ [LF95, SZCO99]. $\mathrm{A}, \mathrm{A}' =$ [YZX96a]. a, a^{*} [GH96b]. A_1 [Min94a]. $\mathrm{A_2B_2} \leftarrow \mathrm{X^2A_1}$ [BJ98]. $\mathrm{A}_x\mathrm{A}'_{3-x}\mathrm{C}_{60}$ [YZX96a]. AgCl^{-} [VABM94]. AgF^{-} [VABM94]. $\mathrm{Al}^{+}(^1S) + \mathrm{H_2} \rightarrow \mathrm{AlH}^{+}(^2\Sigma^{+}) + \mathrm{H}$ [RNS93]. α [FMS^{+}99, HWB97a, JI95, KG98, NSS^{+}95, SWMB94, SST93, VABM94, Woo98]. $\alpha 2$ [VDD96]. α^2 [BSS97a]. α_N [ZLHZ94, ZLHZ94]. as [HHKM95]. Be [OJB77]. β [CFR96, FWZ97, HWB97b, HWB97a, NMSJ99, TCB99]. β_2 [GHB^{+}99]. C_2 [TMD96b]. C_{60} [LRM93, RRC94, YZX96b]. $C_{60}2n$ [LRM93]. $\mathrm{C_{60}NH_2^{+}}$ [TFSZ95]. $\mathcal{L}_{\mathcal{N}}$ [FJR96]. $\mathcal{S}_N$ [FJRS97]. $\cdot$ [MTTS93]. $\cdots$ [CEM^{+}96, SST93, VH96a]. CH^{+} [OJB77]. $\mathrm{CoAl_2Cl_8}(g)$ [DDC97]. D [DBM99, Hos97, MK97a, Flo95, GFRR94, LTSL96a, Mor96a, TV92, BK95]. D_{2h} [Har97a]. δ [LTSL96b]. $\Delta^{-1/2}$ [NS95b]. e [Pai97, PL98, Pai99]. $e^{-} + \mathrm{N_2}$ [PGM95]. η [DMB97]. η^5 [SC98b, SC99]. f [Boe96a, Boe96c, Boe96b, MD94]. $f(r)$ [PZDM97, PZDM98]. g [LBG95, LG96b, LG96a, LG96c]. $GaAs_{1-x}P_x$ [SPFL93]. γ [Bla99, SRP^{+}98]. $h - b - 1$ [GT97, TG96]. H_2 [Cun92]. $\mathrm{H_2N}$

2-dimethylcyclopropanone [CAM+97]. **2-Dithietes** [MF96]. **2-electron** [DWB98]. **2-Hydroxypropanal** [OSA+97]. **2-Hydroxypyridine** [MTD93]. **2-Nitrophenylcyanate** [Mor96c]. **2-Nitrophenylthiocyanate** [Mor96c]. **2-Pyridone** [AL95, MTD93]. **2-substituted-1** [SLG+96]. **2-Trifluoromethylvinyl** [KH97]. **21G** [LJ95]. **21Gsup** [Les92]. **23S** [Voj96]. **273** [RBBL94]. **28H4** [LSC98]. **2D** [LO93, LCP+91, LSGS91]. **2e** [TN96]. **2N** [SES93]. **2nd** [BDC96]. **2NH** [XFF98].

3 [CBT93a, CB93b, CB94a, CFR96, GF94, LJ95, Maz98, MH98, MC95, PVLG93, RK95, SCJK90, SAL+94, TD96b]. **3-21G** [LJ95]. **3-Aminopropionamide** [CFR96]. **3-center** [DWB98]. **3-D** [CB93b, CB94a]. **3-di-** [CAM+97]. **3-dialkylnitroxybenzenes** [TD96b]. **3-Didehydroproline** [RK95]. **3-dienes** [SLG+96]. **3-Diketopiperazine** [PVLG93]. **3-Dimethylimidazol-2-Ylidene** [Cio93]. **3-Dimethyluracil** [PIG94]. **3-Dipolar** [SAL+94]. **3-Isothiazolones** [MC95]. **3-j** [Lai94]. **3-Methyl** [SCJK90]. **3-Pyridyl-** [MH98]. **3-Substituted** [PHBB94]. **3-Triazole** [PGS97]. **31G** [LJ95]. **31Gsup** [Les92]. **3d** [Boe93, Nag96a, Nag96c, RW98]. **3n** [Roo93b, RL97]. **3n-j** [Roo93b, RL97]. **3p** [MTTS93]. **3prime** [NZA92]. **3prime-Azido-3prime-deoxythymidine** [NZA92]. **3S** [BUZ94, WD97].

4 [AAS93, BJMT94, GF94, LGT94, TD96b]. **4-** [BHB+95]. **4-Aminobutanol** [KR93]. **4-Chloro-indole-3-acetic** [RTKP96a, RTKP96b, RTKP96c]. **4-Currents** [AAS93]. **4-Dihydropyridines** [PHBB94]. **4-Diphenylpentane** [LV93]. **4-Nitro-1** [PGS97]. **4-phenylene** [Lah92]. **4-Trioxane** [BJMT94]. **4.2** [RBBL94]. **4.2-273** [RBBL94]. **48** [CAK+96]. **4d** [MS93b]. **4H** [LGT94].

5 [KJL96b, KJL96a, ARdAB95, Maz98, PW97]. **5-** [MSS99a, RA91]. **5-C** [KJ95, RA91]. **5-Contracted** [Maz98]. **5-Fluorouracil** [MRT97]. **5-hexatriene** [HRH99]. **5-HT** [PW97]. **5-Lipoxygenase** [ARdAB95]. **5-Me** [Sta98b]. **5-tetranitroimidazole** [CP99b]. **5-trinitroimidazole** [CP99b].

6 [BHB+95, LJ95, Les92]. **6-21Gsup** [Les92]. **6-31** [FL95]. **6-31G** [LJ95]. **6-31Gsup** [Les92]. **6-Dihydronicotinic** [BHB+95]. **6-Dimethoxy-1** [TD96b]. **6-j** [Lai94]. **6-Thioguanine** [RBBL94].

7 [II94, PMS94]. **7-Cyclooctatetraene** [PMS94].

9' [LK90, LK90, YJL92]. **9'-Dianthryl** [LK90]. **9-Dimethylguanine** [YJL92]. **9-j** [Lai94].

= [ANB94, Ali99, BL99, Bou96c, Bou96b, BZQ95, CB93b, CB94a, GAdAC97, IP93, JKK+92, JH90, Moc99, NG95, NL96a, SM96a, SG96c, SG96b, SGB97,

SGB98, SL97, SC99, SNH99, TST+99, YZX96c, YZX96b].

A. [Kum93b]. **A/T** [LSGS91]. **A2** [ARdAB95]. **AA** [SST93]. **Ab-Initio** [FR92, FR93a, RK91, SKRK90]. **Abacus** [Sri97]. **Above** [CB96a, CB96c, CB96b]. **Above-Threshold** [CB96a, CB96c, CB96b]. **Absolute** [RPB+97, Sie93]. **Absolutrechnungen** [JPD67]. **Absorbed** [DP94]. **Absorption** [AEAO99, AHM97, BJ98, BFV92, BMG+98, Che96, CCZ97, GSSD+96, KLT97, SZ95, WDCA97, LA97, SZ97b]. **Abstraction** [BCS96, Jur97a, YNMT98]. **AC** [SST94, Moi97]. **Acceleration** [Sel93, TMR99]. **accelerator** [Kin99]. **Accelerators** [Hom93]. **Acceptor** [EE91, FKR92, Mor93a, Mor96b, AB99, GBS99, MCT99]. **Account** [MG93a, PTP95]. **Accounts** [PB97b]. **ACCs** [BG98c]. **Accuracy** [JKRW98, JGR98, JMR98, LDP93, LH94, MDM94, Nuñ95b, TNS96a, TNS96b, UWB94, TNS96c, Ber96b]. **Accurate** [Aqu95, BKL97, BLK97, BS95, DLV95, Dun96, Dun97, EJ93, FFD96c, FFD96b, FR93b, IYFI99, JM99, Jur97a, KKT93, KLLI97, MHL94, NB93, Nuñ94a, SGGC99, Sim98, SLD95, Tas93, Taş96a, BSS97a, FFD96a, New97, NL96b]. **ACE** [Ish96]. **ACES** [SGW+92]. **Acetaldehyde** [ADPS98]. **Acetaldehyde/Vinyl** [ADPS98]. **Acetaldimine** [ADPS98]. **Acetaldimine/Vinylamine** [ADPS98]. **Acetate** [STS95]. **Acetic** [FT95, FT96, FT97a, RTKP96a, RTKP96c, RTKP96b, RT99, RT98]. **Acetone** [MR92, PBB92, DV96]. **Acetonitrile** [MDD93]. **Acetyl** [RK95]. **Acetylene** [FF94a, Fou94, Jur99a]. **Acetyloxyl** [KVS98]. **acetylpropanamide** [ZH99a]. **ACh** [WJC+98]. **AChE** [WJC+98, WJC+99]. **AChE-catalyzed** [WJC+98, WJC+99]. **Achieving** [MVS97]. **Acid** [AP93, AP96, BKEMM94, BAK97, BHB+95, CLR+93, CFR96, DM95, FT95, FY95, FR92, Flo95, GJLA99, KE91, Les92, LX95, NSS+95, PHBB94, RFG99, Ram90, Ram94, RTKP95, RTKP96a, RTKP96b, RT98, SPG97, SHC+98, Tew94, YW92, FT96, FT97a, HWB97a, KK99b, LHNK99, RTKP96c, RT99, SSM+99, Tew97, TFR99, TBP99]. **Acid-Base** [SPG97]. **Acidic** [BKR97]. **Acidities** [BMP93, MBP91, RPB+97, SSN99]. **Acidity** [PLG95]. **Acids** [AHM97, BDG96, BKWL97, CLC90, MBP97, HWB97b, KKM99, MKBP97]. **ACPQ** [PTP95, PTP95]. **Acrylonitrile** [HDY+91, MMA+92]. **Action** [JGCJ96a, JGCJ96c, WD91, JGCJ96b]. **Activated** [NP96b]. **Activating** [DAF+96]. **Activation** [CBSR+98, Cun92, CC96, Jur97a, MÅ99b, MC94, PW97, PVU+93, RR94, RNS93, Sak98, ST96b, TWK+92, BYE+97, FMS+99, PBS99, SC98b, SC99]. **Activation/Cyclization** [MC94]. **Active** [EBG95, HM99, KM90, KN99b, KW98, KSK91, NK98, SBIP97b, TKK+90, VC92, GFGB99, KK99a, KN99a, MHY98, SZCO99, WWFR99]. **Active-site** [HM99, GFGB99]. **Active-Space** [EBG95]. **Activity** [BBE95, FT95, GJOV97, HB94, Khu92, Lev94, NHN97, NZA92, PW97, Pul90, RFM90, Reg92, SM94, SC96a, SC96c, TBBE98, ZCT98, BTKVG99, Bha99, CMA+99, FT96, FT97a, SC96b]. **Actually** [Sta98c]. **Acylation**

[DDP96, SCA93, WJC+98]. **Acylhydrazones** [DDRB96, DAR+96a, DAR+96b]. **ad** [And93b]. **Adaptation** [PKJ99]. **Adapted** [CDDM96, Flo97a, JPJ95, JM99, KPR97, LP93, MPKR94, NU95, PRTV97, PTP95, RPKM95, VLCBPR97a, CLZ99, Flo97b, JRS+99, LV97, MD99, PC99, VLCBPR97b, ZWD98a, ZWD98b]. **Adatom** [SD98]. **Addendum** [Csa90a, Mey97]. **Addition** [AMKS93, ET97, HWS92, OSA+97, YTYS97, TFR99]. **Additive** [Lev97]. **Additivity** [May92]. **Adducts** [FW92a, FW92b]. **Adenine** [HB95, MKM93b, Tew94, Tew97, LF90, SSM+99]. **Adenine-Thymine** [LF90]. **Adiabatic** [GL95, HL79, II94, KC98a, Nag95a, PY92, SB98, STMR97, CSG99, KLC98b, OKY+99]. **Adiabaticity** [Lef97]. **Adjoint** [KE93]. **Adler** [Deu96]. **adrenergic** [FMS+99, GHB+99]. **Adrenoceptor** [TWK+92, WD91, WTDB94]. **Adsorbate** [NNMH96, HS99]. **Adsorbates** [DDH+96, Hea97, Kun90, PSBL98]. **Adsorbed** [GMR+93, JAG95, LLZ98, MVB92, SM99]. **Adsorption** [JSG97, MD91, NTL96, Bre99, CPD+98, HS99, MCS98]. **Advances** [KPD93]. **Advantages** [FFD98]. **Affinities** [BHKK93, CA97, DS90, GKKM96, Jur97g, KCLI95, NKUS97, PD93, STMR97]. **Affinity** [BDG96, GJLA99, MMA+92, RB93, STC96]. **Aflatoxin** [WP90]. **AG** [SST94, Ali99, CBAM97, KSN93, ANB94, NHN97, NKUS97, SNH99]. **Agent** [BVV91]. **Agents** [BHV96a, BHV96c, DDRB96, DAR+96a, WTDB94, BHV96b, DAR+96b, WWFR99]. **Aggregate** [DP93, DS99, NYNY99]. **Aggregates** [NY98]. **Aggregation** [LL94a, MDD93]. **Agonist** [VDD96, WD91, WTDB94]. **Agostic** [JKK+92]. **AGP** [Col97]. **Agreement** [TGDS97]. **AH** [BCY95, BCY95, NBS95]. **Aid** [FSHC99, Jac97, Jac98]. **Al** [SRP+98, Bau98, BCY95, BZQ95, DFL98, DLF99, HS99, KJ97, LMC97b, MVS97, MBML91, TIPM96]. **Alanine** [Ram90]. **Alberte** [Ano99a]. **Alcohol** [ADPS98, CAK+96, RAM91, Ryd94, KH97]. **Alcohols** [BSP97, SSN99]. **Aldehyde** [SSMK93]. **Aldehydic** [VBUS99]. **Alder** [Bra97b, MV98a, SLG+96]. **Algebra** [Alt96, CP92, Jon92]. **Algebraic** [AB96, CXFP99, DlD99, FC99, GMI95, GYDY97, ILL96, IP93, KKT93, Lai94, Lin81, MPSLB91, Réc90, RJ92, SM96c, WMP69, CVP90, GDYY97, Jør92, Sim99c]. **Algebrants** [Pos91, LP97d]. **Algorithm** [Cul95, HO94, Ish96, SB98, Sel93, ST96a, TCM98, WWM+98, ZDO96b, ZDO96c, HVS98, MVHV96, ZDO96a]. **Algorithmic** [Lio92]. **Algorithms** [FGRS98, Pos91, PR97, Roo93b, ZO94, ZO95, ZDO99]. **AlH** [CWJ+99]. **alignment** [Ata97a]. **Aliphatic** [CLC90, SSN99]. **Alkali** [Bat92, BRS95, BK94c, Csa94, LRM93, LRM97, MLR+98, YZX96a, YZX96b, YZX96c]. **Alkali-Doped** [LRM97, YZX96a, YZX96b, YZX96c]. **Alkali-Semiconductor** [Bat92]. **Alkaline** [Csa94, DTA+96, KPTS94, LRM93, STS95, Sta98c, TSS95]. **Alkaline-Earth** [DTA+96]. **Alkaline-Earth-Intercalated** [Sta98c]. **alkaloids** [Bha99]. **Alkane** [CD90, WGRM94]. **Alkanes** [Gin95, Gin96b, MK98b]. **Alkenes** [ET99]. **Alkoxo** [CdBKZ99]. **Alkoxo-Bridged** [CdBKZ99]. **Alkyl** [FLF96].

HDB+95, IK94, JM95, JM96a, KFS92, KBT94, KRZ91, KKE+96, KL97b, KL97a, KCLI95, LJS94, MK90, MM94, MR92, MD93c, Nag96a, Nag96b, Nic99, NV94b, NS93b, OJB77, PM93, RVP92, SCL96, SDW+98, SZL95, SZ97a, SS99b, STY+98, Sim95, SSM90, SGGMGFS96, Ste96, SATP94, TNSM99, TMSI98, TC98b, VH96a, WP91, WA94, CM99, HC96b, MRC99, Ort97, SN99, vG96, SOK+98, TGS99, Wil99b, BTKVG99, CCWCF96, KLC98b, LKM99, LV97, Nag96c, NYNY99, NV97a, TC98c, YB99, ZPBC97].
Applications
[ADB96, CWZ98a, Ced90, CVW91, Del92, DQB97, Enk97, GP95, GG97b, GLBM96, Hom93, JL70, Kup98, LLC+94, MPR97, NS93a, O'C96, PEBS97, SM96b, SB96, TZ97a, Wil96, ZM95, ZLHZ94, LBL98, Ort98a]. **Applied** [BLE96, BČ96b, CFMA95, CJH98, ČB96d, Dau94, KD98, KPTS97, LCLO95, NPL90, PDT97, RDK97, Roz97, Sta93, VJ95, VJ97, AZ99, Cze99, FR98, HMK99, RDK02]. **Approach** [AB96, ÁC94, ATI97, AM90, AO93, Ave79c, Ave79a, Ave79b, Ave80, ABLA97, BA91, BM96, CLZ95, CLSI94, CG96, Csa90b, DlD99, DFDK99, DC95, Del98, Dew92, DB94b, FK94, Fer96, FFD98, FBKD97a, FBKD97b, FBKD97c, Flo97a, Fri93a, Fri93b, FDD95, GJ95, GD94, GSD97, GGSA98, GYDY97, GNA98, Har71, Har97b, Huz96, JPJ95, JZ95a, JZ95b, Jur96a, KSR95, KNA94, KPTS94, KPM+90, Kry98, Kup98, LY98, LP96, LD95, LBBE98, MKM93a, May98, Min90, MKM96, MAPLB92, MPJ97, MPJ98, MV92, MSCP92, NY98, Nic96, NS92, NS93b, OJB77, Pal97b, PY92, PPP97, Pic92, PC95, PB95b, RP96, RK91, RMF90, SA96, SAR96, SM96c, SCP91, SG94, SGGMGFS96, SLD95, SP94, VD90, WLBL94, WP95, XY95, Yu95, CPA98, Flo97b, FJR96, GDYY97, KKS99, Kin99]. **approach** [KSW98, LF99, MM99a, Mar99a, NYNY99, NM96, OKY+99, PFK99, SK99a, SGK99, WG99, Wil99a, YUSM99]. **Approaches**
[BA97a, BBC+96a, BAK96a, Chr97, FGRS98, FWC+93, JOC97, NB97, PTP95, RZ96, RWT91, RWT92, CGG96, HBGR99, Mat97]. **Appropriate** [Gin95, MYN+96]. **Approximants** [CG95, CB93a, GB71, LBPL97]. **Approximate** [BMA99, CV94, Fer95, HHKM95, KS98, Mez97b, NP96a, Nuñ95b, Ort98a, Ort99, PTP95, Rin96a, Rin96b, SDW+98, CVP90, Rin96c]. **Approximately** [SFM94]. **Approximating** [TNI96a, TNI96b, TNI96c]. **Approximation** [BKR97, Bec94, BPE97, CM96a, CFMA95, Che93, CC97a, GRB+93, GVB97, Hag97, KS94a, Kir95, KLLI97, LLC+94, LP74, LL68, MJS93, MV99, NS95a, Ney95a, Ney95b, NI94, ÖL78, PP98a, RRC94, SZ96, Sha95, STY+98, SBIP97b, SS91, SS92c, Spe71b, VZ93, ZDO96b, ZDO96c, ZC95, AZ99, BDPS97, Kün99, NM96, SNNY99, TGS99, YB99, ZDO96a]. **Approximations** [BAD99, DP97, GvLB96, Kas76, KP75, LV98, LP94, Sah95a, SN90, Spe72a, TP90, TK92, HC96d, KPB99]. **Aquatic** [ML97]. **Aqueous** [BHH92, BMP93, DV91, JI95, MBP91, SM98, SWK90, AGAP98, AFM99, ESHP99, NOY98]. **Aquifer** [Har97b, Har98b]. **Ar-HCO** [DQB97]. **Ar0** [II94]. **arabolicity** [EC96a]. **Arbitrarily** [TTOY93]. **Arbitrary** [GSM90, Kat98b, KPA95, LS93a, LDP93, PS96, BSS97a]. **Architectures** [KJdL+93]. **Area** [Art98, KM99a]. **Argon**

CXFP99, GT97, SSM+99]. **Basic** [BKR97, Jac92, LMD96, Spe71a, HC96a]. **Basicity** [BK94c, PZTPMC99]. **Basis** [AHI96, AMKS93, AHWA96, BC96a, BL72, Boe96a, Boe96b, BR94, BEJ98, Bro96a, Bro96c, Bro96b, BDH+97, CM96a, CHM95a, CHM95b, CHMA95, CSS93, Cul91, Dat95, DBLV94, DLV95, Fer96, FFD98, FR93a, Flo97a, Gin95, GT93, HH97, Hil98, HS91, HS92d, HS92c, Ish91, Ish92, JEB92, JM99, Jur98a, Jur98b, KSR95, Kas76, KKT97, KH95, KYW95, KL97a, Kru92, Kut94, LJ95, Les91, LTP96, LO90, Löw67a, MSS95, MHS95, NNMH96, NE95, PG94, Pah98, PVLG93, PHH94, Pen93, Pen96, PMN+92, PCCO94, PDT97, RPJZW96, Sad97, SPOAS97, SA96, Sur94, Tal93, TZ97a, Taş97, Ter97, TJ95, TKSH93, US97, UBA92, VCCM92, VAVN91, WSW96a, WSW96b, Wil96, YNO94, Bla99, BC97b, Boe96c, BSP98, BGS97, BG98b, BG98c, BG98d, Flo97b, FR98, ISOA99, JRS+99]. **basis** [KH96a, Lon99, vMVvLvD97, PKJ99, PB99, RAI99, Sta98d, WSW96c, Wil99a]. **Basis-Set** [CHMA95, PHH94, WSW96a, WSW96b, PB99, WSW96c]. **BaTiO** [AMC97]. **Bay** [KL93a, vS95]. **Bay-** [KL93a]. **bcc** [MESH93]. **BCS** [Aon98, PC95]. **Be** [JM95, REL+90, TST+99, CL94, CDDV93, Löw94, Sta98c, BSHP97, BKL98, JM93a, JM96a, KP97, LBG97, RA96, RKPE95, FMD+96]. **BeC** [DTA+96]. **Becke** [Jur97a]. **Become** [Klo90]. **BeFH** [ASP97]. **Beginnings** [LFB96]. **BeH** [CAJ95, SL93, SGGMGFS96]. **Behave** [ATP+96]. **Behavior** [BE98, BHX96, DS93, GBRA94, LTSL96c, LTSL96b, LTSL96a, Núñ96, PV98, TKMA92, WSW98, YUSM99]. **behind** [Kry96]. **Being** [Klo90]. **Beings** [Fuk95]. **BEM** [DV91]. **Benchmark** [Jon93, Tri97]. **bend** [NMSJ99]. **Bending** [LSGS91, Sen96]. **Benoxaprofen** [dAdM95]. **Bent** [OCK99, DV99]. **Bent-bond** [OCK99]. **Benz** [KL93a]. **Benzaldehydes** [SSMK93]. **Benzene** [CCZ97, Oli99, Thu69, VH96a, YNO94, CVP90, DV99, GZSvD99, VLCBPR97b, Vin92, Cio94]. **Benzene-Tetracyanoethylene** [Cio94]. **Benzenes** [Cha97, MG93b]. **Benzenoid** [GRK96, HGP+92, Ran97, Gut99a, RG99]. **Benzo** [KL93a, WP92]. **Benzocyclobutadiene** [KGC+96]. **Benzocyclobutadienes** [KEMM93]. **Benzocyclobutenes** [KEMM93]. **Benzodiazepine** [GVV+90, VL91]. **Benzofuran** [PMJM+91]. **Benzohydroquinone** [DM95]. **benzoic** [HWB97b, HWB97a]. **Benzoyloxyl** [KVS98]. **Benzylidene** [METHH94]. **Benzylimidazole** [VDD96]. **Bergman** [BS95]. **Bernard** [Ano99a, Ano99e]. **Beryllium** [Boe95, MFP96, MV90, Mor94, PZ95, LBL98]. **Bessel** [TZ97a, TZ97b]. **beta** [Ram90, LCP+91]. **beta-Alanine** [Ram90]. **beta-Spiral** [LCP+91]. **betasub** [TWK+92, WD91]. **Bethe** [Por97, Por98, Por99, PR97]. **Between** [Aon98, BBC+96a, BLBP97, BP93b, BP93a, BTN98, BPL97b, BL92, Bra97b, BHV96a, BHV96c, Coo94, CE90, DM93, Del96, FF94a, FF94b, Gal72b, GG97a, Gin97, HP97, Iga95, JTZ+96, JBT+95, Jur98a, KBA96, Löw95b, Löw99, Luk92, Mar97a, MW68, ML97, Mon98, MPJ98, MBP97, NYY96, NK96a, OHSF97, Pie93, PS94a, Pro95, Reg92, RML97, RRS97, RW92, SF95b, Sch99b, Scu95, Sla67b, WGRM94, YW92, AGM99, BBTU97, BHV96b, CZ94a, CWJ+99, GFGB99, GDYY97,

RA91, SC98b, SC99, YZX96c, AS99, BL99, BBZ91, BSS+97b, CCC+95a, CD93, CXFP99, CL92, DM98, DM99, EDF+98, GS93, GS97b, GAdAC97, HRRBL97, HZ94, HOF+97, HL93b, JM93a, KP96, KH96a, LFS94, LL99, LSC98, LCS98, MLL99, RG99, RN96, RA91, SK99a, SCA93, Sel93, SLA97, SZCO99, TST+99, TPR96, TFSZ95, TZCT97, Thu69, TMD96a, TMD96c, WYW96, XY95, YZX96a, YZX96c, JTZ+96, MPSF97]. **C-** [SCA93]. **c-BN** [MPSF97]. **C-H** [HZ94]. **c-Myb** [JTZ+96]. **C.** [Jen99]. **CA** [SST94, BC97b, CCC+95a, Pro95, YDDP92, WZ99]. **CaC** [DTA+96]. **Cadmium** [LMMK93]. **CaFsub** [LW92]. **Cage** [BBZ91]. **Cages** [ZSK97]. **Calais** [Löw96a, Pau97]. **Calcium** [BPL97b, WLBL94]. **Calculate** [CE90, MMA+92, MIW91, ZLHZ94]. **Calculated** [CHMA95, CGRB94, DE92, Dat95, FR93a, HS95, KD95, LV98, LH94, RRC94, YLLJ96, SNH99, BHKK93]. **Calculating** [ACAT92, CZ94b, CB96a, CB96c, Coh97, DZO97, HZ99, JM96b, Roo93b, SF94, Val96, CB96b]. **Calculation** [ASP97, AL98, ALRP96, BLB95, BB97b, BL92, CJA94, CS96a, CS96b, CCZ97, Csa90a, Csa91, DDG93, DKTZ94, DV98, DZ96b, DB94b, ETV94, FCVL98, FGM90, GSD97, GMI95, Har97b, HU94, Iga95, Jas94, JR96, Jon97, JM96c, KNN96b, KNN96d, KKNN97, KSY97, KPTS94, KLT97, KCLI95, KSK91, Kur90, Lev94, LTP96, LP74, LD94, LR94, LL70, LS92b, MHÅ98, MHS95, MBA97, Mez94a, MVV+97, MAD98, MGLBP95, Mor96b, MD93b, PSAUS90, PVLG93, Pen93, Pen96, PMN+92, RN96, RPB+97, RL97, SM96b, SBM97, SSO+97, SZ96, SZ97a, SCP91, Sem96a, Sem96c, Sem96b, SSMK93, SATP94, TSPKM94, VMCK97, WD97, Wen93, WL92, WR96, WZ99, YNO94, YLD97, YBZ92, ZZW94, ZW96d, BKL98, CS96c, DD97b, KNN96c, LLB99, MRC99, SAW97, SN99, SSN99, TTM99, Tit96]. **Calculations** [AHI96, AH97, Ave79c, Ave79a, Ave79b, Ave80, BL77, BBZ91, Bér97, Ber96b, BNLF96, BT96a, BT96c, Boe92, Boe95, BBC92, BB94, BB95, Bou96a, Bou96b, BEJ98, BPL94, Brä68, BW90, BS92, BS94, BCY95, BJLK98, BL98, CM96a, CMF+98, CHM95a, CHM95b, CHMA95, CCC93, CZ94a, CA90a, CMA93, CFB97, CM94a, CLKMTA95, Cul95, DHLS94, DREW98, DRBE96, DO90, Dun96, Dun97, EP98, Egu96a, Egu96b, Eld73, EMMS94, EJ93, Fer96, FFD96c, FFD96b, For94, GKKM96, GDID98, Gal72b, GMS97, GS68, GRT96, GT93, GPD94, Gre94, GP97, HMGP93, HSLL92, HLS94, HBL99, Har71, HNB92, HMLK98, HC96e, HZ94, HW91, Hua92, IANK94, Ish90, IK97, Jac97, JCÁ96, Jen94, JH90, JL70, JAG95, JSG97, Jur96a, KLLB98, Kar98, KP75, KS98, KBL95, KKL90]. **Calculations** [KF96a, KF96b, Kol97, KK93, KA95a, KYW95, KL97b, KL97a, LGBL94, LMC97a, LP97a, LRM96, LMMK93, LBM94, LY98, LS67, Les91, LHL91, LW92, LFS94, Lin92, Lin96, LCLO95, Loh91, LL92, MYN+96, MSS95, Man95, MF96, Mar95c, MW92, MGNK95, MH68, MLK94, MAI95, MSCS95, Mor93a, Mor97b, MNC95, NPL90, NV94a, NV94b, Núñ97, NV97b, Oku98, Ort98b, PCE95, Pah98, PS68, PNB94, PK76, PK77, Pra97, RC92a, RTKP95, ROL+90, RC92b, RML97, RSD97, Ryd94, STKN90, SB95, Sas74, SO94, SCMF93, SHF94, SBAD90, SNMB97, SPF96, SB90, SRS92, SG93, SST93, SST94, SR96, SBIP97b, SLA97, SBD+92,

SAL+94, vH96b, Sta95, Sta96a, SL97, SDG97, SPR94, SJ91, SJR91, Tal93, TJ95, Tos95, Tri97, VABM94, VV95, VIK98, VAVN91, WD95, WZW96]. **Calculations** [WB94, Wen96b, Wen96a, WP90, Wil96, YNY99, ZO94, ZO95, ZC95, dVJ93, AMC97, BK97, Bla99, BT96b, Boe97, BJA99, Bou96c, BB97a, DV96, Egu96c, ELMY96, FWS97, FFD96a, Gur99, HR99, HS99, Jac98, KLO+98, KH96a, KKNY99, KF96c, LMC97b, LFD99, LBL98, LXWZ99, MKRW99, MVS97, MECE97, MSS99b, NV97a, Ort98a, Ort99, PWL98, PSBL98, RP98b, SGGC99, SEKEB98, Sta96b, Sta98d, Sta98e, SZ97b, Sut99b, ZDO99, ZWD98a, ZWD98b, Van96, vMVvLvD97, SJ97, WGP99]. **Calculus** [Kin96, Ney95b]. **Call** [Ano98b, Ano98c, Ano98d, Ano98e, Ano98f, Ano98g, Ano98h, Ano98i, Ano98j, Ano98k, Ano98l, Ano98m]. **Callaway** [Tri95]. **cam** [CL90]. **Camphor** [CL90]. **Can** [Bau98, GVK99]. **Cancer** [LFB96, Lad97a]. **Cannabinoid** [RFM90, Reg92]. **Cannabinoids** [PHBB95]. **Canonical** [FK94]. **capacities** [NOY98]. **Capacity** [Pal93a]. **Capping** [ZLWES99]. **Capture** [BMA93, BF96, KSW98, SK99a]. **Car** [Kry93]. **Carbanions** [OKI98]. **Carbene** [Cio93, Sak98]. **Carbenes** [SG97, SGB98]. **Carbides** [SGB97]. **Carbon** [AMRT94, AMKS93, BKS96, BF95, KL94, MR92, Suh93, TAY+97, VMCK97, WTSN94, XR94]. **Carbon-** [Suh93]. **Carbon-Carbon** [BF95]. **Carbonic** [BAK97]. **Carbonyl** [ET97, VBUS99, GS97b]. **Carbonyls** [SZL95, SG96a, SG96b, SG97, SGB98, MSMR99, SG96c, Van96]. **Carborane** [RA91]. **Carborane-Hydrocarbon** [RA91]. **Carboranes** [PK77]. **Carboxyl** [KVS98]. **Carboxylic** [MBP97, MKBP97]. **carbyne** [DM98, DM99]. **Carcinogen** [WP90]. **Carcinogens** [LP97b]. **Cardiac** [MBV+98]. **Career** [Kas99]. **Carlo** [ACB+99, ACAT92, ACHT95, BBMM99, BBC+94, BBC+96b, BRA+99, BRV99, Cor97, CDC98, KNN96b, KNN96c, KNN96d, KKNN97, KI94, Kid99, MB97b, Rey90, Rot96, Rot97, UBA92, VBD+98]. **Carotenoids** [TCM98]. **Carriers** [LTSL96c, LTSL96a, LTSL96b]. **Cartesian** [Sch92, KA95b, Le 97, SF95b]. **CAS** [PPP97, YNY99]. **CAS-SCF** [YNY99]. **Case** [BA91, CT95, LB96b, LB96d, RRC94, BBMM99, LB96c, MVS97, PCD99, SC99, TMA97, Whi99]. **cases** [hJH97]. **Casimir** [Mon94]. **CASMP2** [YTYS97]. **CASPT2** [BBC+96a]. **CASSCF** [BBOR96, BBC+96a, GMMH97, LHNK99, MCOS94, Pra97, SG93, XLW+99, YTYS97]. **CASVB** [CTG97, TC98b]. **Catacondensed** [Ran97]. **Catalysis** [FB96, MÅ96, SNMB97, SPG97, Tch96b, KÅ99]. **Catalysts** [EZ93, SDE94]. **Catalytic** [CJX+92, EZ92, HBH98, NHN97, PB95b, Ryd94, DD99, FNSV99, GWB97, XYC98]. **Catalyzed** [BT96a, BT96c, PHBB94, SJ91, BT96b, KKS99, WJC+98, WJC+99]. **Catastrophe** [MS90]. **Cathodic** [HDY+91]. **Cation** [AKD96, BLC95, GKKM96, GMS97, Jur99a, Yam97, Gal98, YNNR97]. **Cationic** [Bou94, FW92a, FW92b]. **Cations** [BSHP97, HDB+95, LE92, MKM93b, Pro95]. **Cauchy** [BOX94]. **Caused** [TMDB98]. **causing** [Hag99b]. **Cavities** [PB95b, RPJZW96, ZWJP95]. **Cavity** [CDD+99]. **CBC** [KJ95]. **cc** [GR95a]. **CCCH** [CMF+98]. **CCD**

CA97, Csa90a, Csa90b, Csa92, CB94b, Dau94, DPPM94, DZ94, DD98b, DZ96a, DA91, Dob98, DDC97, DKBB97, Dun96, Dun97, EDH$^+$92, Eng95, EMMS94, EMMS97, FEE$^+$98, FP94, FT97b, FWC$^+$93, GMS97, GR94, GR96a, GG97a, Gho94, GD94, GSD97, GD96, GWB97, GJPF92, GRBA92, GBRA94, GNF90, Gör98, GPD94, GG97b, Gre94, GWCT97, GLBM96, GK91, HMGP93, HCR94, Hag97, Har71, HK95a, HLJ96a, HLJ96c, HHKM95, HM95, HM97b, HBH98, Jac97]. Density [JBT$^+$95, JH90, Jou97, JZ95a, JZ95b, JM96c, Jur96a, Jur96b, Jur97a, Jur97b, Jur97c, Jur97e, Jur97d, Jur97f, Jur97g, Jur98a, KLLB98, KBGE97, KBWJ96, KVB97, KS94a, KBA96, KD98, KS94b, KVS98, Koh95, KMM96, KL97c, LS71, LZ96, LY98, LP94, Lev97, LLZ98, LKLBP98, LL70, Lu99, LLBM$^+$95, LAS$^+$95, MG97, Mar92, Mar94b, Mar94d, Mar95b, Mar95a, Mar98b, Mar98a, MRT97, MFP96, MSMR99, Maz98, MB98, MESH93, Mez97b, Mic96b, MDJ98, Min90, Mor93b, MCA95, MNC95, MSCP92, Nag94, Nag98a, NV97b, OGK90, OHSF97, PCE95, PSAUS90, PP98a, PMDM97, PZDM97, Per98, Per93, PB96, PEBS97, PRTV97, PG96b, PG96c, PNB94, PGS97, PSCZ97, PAAM98, PK96, PS94b, RL95, RPKM95, RVP92, RHC96, RPB$^+$97, RDK97, RP98a, RSD97, RRS97, SPH98, SH90a, Sam97, SPOAS97, SDW$^+$98]. Density [SSO$^+$97, SF95a, SD97, SPC96, SZL95, SZ96, SZ97a, Scu95, SCP91, SP92, SCP93, SPT96, SPSZ96, SPSMZ96, Sha95, STY$^+$98, SNNY99, STMR97, SR96, SCS94, SS91, SLM70, SFM94, SMO$^+$96, SAL$^+$94, SG96a, SG96b, SG97, Spe71a, Spe71b, Spe72a, Spe72b, vH96b, Spr93, SLD95, SDG97, SC99, SATP94, Suk94, Suk95, Sur97, TKNI96, Tac96, TC98a, Tet93, TP90, The94, TG95, The97, TSPK96, TSPK97, TB95, TCM98, Tri97, Val94, VB94, Wlo95, WR96, YNY99, Yor95, YNNR97, ZC96a, ZC96c, ZC96b, Zap95, ZY94, Zie96a, Zie96b, ZC95, ZPBC97, Ali99, BDPS97, CCS98, CP99b, CMA$^+$99, CEM$^+$96, Cze99, GSKC99, HLJ96b, Hol98, Hud99, Jac98, Jur99d, Jur99c, KK99a, KC97, KPB99, LCB98, LBL98, MHN98, Mar99a, MVS97, MECE97, MLL99, MR97, NYKY98]. density [PMDM98, PG96a, RDK02, SN99, vG96, SPM$^+$96, SG96c, SNH99, TNSM99, TC98c, TGDS97, VVO98, WW97, WGP99, WMZ98, YB99, ZTC97, Zie96c, Van96, Mar99a, PMDM98, PZDM98]. Density-Dependent [KLLB98, Scu95]. Density-Functional [Cal93, CZ94a, Csa90a, Csa90b, Dun97, EDH$^+$92, GNF90, Gör98, GK91, HCR94, Hag97, HK95a, MNC95, PSCZ97, SH90a, SPOAS97, SCP93, SS91, Spr93, Tet93, The94, Yor95, MG97, CCS98, TC98c]. Density-gradient [ZPBC97]. Density-Gradient-Expansion [SS91]. Density-Matrix-Response [TCM98]. Deoxyadenosine [KJL96b, KJL96a, KJL96c]. Deoxymyoglobin [GSSD$^+$96]. deoxythymidine [NZA92]. Dependence [CR93, EPB97, FP96,

FMDA94, FR93a, FDAC90, GLLY94, HSWS95, KSH94, MPV94, MBA94, SC98a, FV96, LP99, MJLL99, MPIP99, PB99]. Dependencies [Boe92, YNNY99, vMVvLvD97]. Dependent [ASI94a, AV92, AM97, Bec94, BFL91, CT95, CT96, CSP98, DFDK99, DD98b, FBKD97c, Gör98, JR96, JL70, KLLB98, KSY97, KCLI95, Löw67a, LG95b, Mor96b, PG96b, PG96c, RB95, RW98, Rod91, RMF90, SB95, Scu95, ST93, TC98a, TCM98, Tri97, BMA99, CCS98, GBS99, Lon99, PG96a, TC98c, YB99]. Depleting [DP93]. depletion [BH99]. Depopulation [KSK+99]. Deposition [AST95, CL95]. Depositions [WTSN94]. depth [MCB99]. Depths [PB95a]. Derivation [Bro95, HWS92, KC98a, Sah95a, HC96a, Hos97, MD99, Vin92]. Derivative [KSY97, MK97a, Sem96a, Sem96b, TSPKM94, Sem96c, Tho96]. Derivatives [AST93, Bra97b, BHB+95, BBE95, CCM+96, CTC95, GBVM93, GKKA97, GJLA99, HDY+91, Jou97, Kin96, LB94, LSC98, Lu99, MS98, MH98, MV99, NdA93, RAM91, SSK+92, Sza95, TBBE97, TBBE98, TSRP99, VDD96, WB93, LCS98, SZCO99, SSM+99]. Derived [FF90, HPSC97, JBT+95, KKL90, KY93, Roz97, PLBB99]. Dermal [MK96a, MK96b, MK96c]. Describe [Bau98]. Described [DZF93, GSM90]. Describing [BA90, Sza95]. Description [BUZ94, GVV+90, Hed95, KGC+96, KMM96, MKM97, NP96b, Per98, PS99b, Ryl99, Sch99b, dSdSN95, Tom91, DBM99, Nal98, YNNR97]. Descriptions [Cio94, Loh96, Mar95c, TC98b, VdV96]. Descriptor [Kin93]. Descriptors [Art98, BDG96, KRB+97, MRBO96, MRB+96a, RD98, MRB+96b]. Design [ARdAB95, KPM+90, Ott94, RC92b, San97, SHBS96, SHB+96a, WL67, ZCT98, SHB+96b, WWFR99]. designing [AI99]. Desorption [MD91]. Destabilization [MSP94]. Detachment [DZO97, RB93]. Determinantal [Csa93, Cza95, TM93]. Determinants [Iga95, PVU+93, WB94]. Determination [BK96, BFH96, CMFA93, CL94, DM95, DS90, DZ94, GL92, Her97, KCI98, MTNF99, MS97a, OJB77, PNB94, Sch93, VJ95, VJ97, WDD93, KK99a]. Determine [Hag98, Su93, Tos95]. Determined [BDNT97, PSO90]. Determining [HZ93, Maz98, PRVS95, XY98]. Detour [TNM97]. Development [BAF+95, GSM98, Her98, Löw95a, Löw97b, MBV+98, MPOG99, SSO+97, ST96b, Sut96]. Developments [BD95, Jon94, LJN+98, Ott94]. Deviation [Gui98]. Dewar [Ano92a]. Dexanabinol [PB97b]. DF [GGSA98]. DFT [SPF96, AOH96, AHI96, BBTU97, BLE96, BBC+96a, BT96a, BT96b, BT96c, Boe97, BTN98, CCS99, Dav98, GFY+99, GS97b, GL95, GJDD97, Gut99b, hJH97, Kün99, MB97b, MPJ98, NL96b, Pra97, SC96a, SC96b, SC96c, ST97, SGB97, SGB98, TSP97, VV95,

[AT93, FLHT90, FWBT94, Her98]. Dynamics [ABB93, ADB96, Ata94, Ata97b, BS93, BA91, BTTS97, BM96, BCMÖ97, BSHP97, Brä93b, BFL91, BFV+93, CN94, CD93, CFB97, CCT98, DHLS94, Deu98a, DD98a, DD98b, DÖ94, DKBB97, Dun98, EE91, FWT+96, GBS+93b, GH99, GGHP94, GLBM96, GW98a, HGC93, HL93a, Hop90, JO94, KDHW90, KYW95, KMM96, LLC+94, LMD96, LKU90, MHÅ98, MY99, MK98b, Nag96a, Nag96b, NY98, Nic96, OMTS97, ÖOD96, Oku98, PY92, PTC94, PPSK96, PPK97, PP98b, RB95, SB95, SB97a, SB97b, SHF94, SNMB97, SCP95b, SD96b, SM92, TW90, The94, TBW90, Tul91, WLBL94, WGRM94, ZA95, ZZCSE94, Ata97a, ESHP99, GVK99, HM99, Hag99a, KJ97, Kry96, MCB99, MJLL99, Nag96c, RC99, SKC99, TCB99, Tho96, TMR99, WGP99, Kar96]. Dyson [SS98, TMD96a, TMD96c, TMD96b]. Dyson-corrected [SS98]. DZP [JG95].

e-Doped [LTSL96c]. e-N [MM94]. E. [Kar96]. E/p [TSPKM94]. EA [Bau98]. Early [SL93]. Earth [Csa94, DTA+96, LRM93, Sta98c]. Easier [BAF+95]. Eclipsed [Pal94]. ed [BDC96]. Ed. [Mic97]. EDA [SBM97]. Edge [BSS96, CF96, ML99]. Edge- [CF96]. edge-to-loop [ML99]. Edited [Ber96b, Enk97, Eri93, Kar96, Mon93, Sta93, Mon94]. Edition [Str93]. Editor [Mat97]. Editorial [Löw90a, Löw90b, Löw91, Löw92, Löw93a, Löw93b]. Effect [ADB95, AMKS93, ABDM94, BSS96, Bau97, BN74, Bre99, BLG95, CHMA95, CEZ+99, CL90, DB94a, DZ96b, EC96b, EC96a, EBMS92, FLF96, Gao93, GSPSM93, GMS97, GH99, HGP91, KUN+98, KEMM93, MV98a, NK96a, PSD97a, PAC98, PM93, SKJ98, SY91, SIM93a, SS92b, Sri97, ST96b, TG96, Wan94, WBD97, Xu96, ZLWES99, vS95, Aon99, EC96c, ISOA99, KA96, vG96, SLG+96, WW97]. Effective [Ara94, BAR94, BCLS94, Bra75, Coo95, CPTR96, CL94, CL95, FDD95, FD96a, Gin97, GG97b, GvLB96, HS93, KFS92, KPTS94, KA95a, MTL97, PG94, Pai97, PL98, Pai99, Sch99b, SR96, STM96a, SJ97, Tom91, YBZ92, BC97b, CB99, DP96, KLO+98, RCB+99, STM96b, TM99, TC98c, Van96]. Effects [AL95, Ata94, Ata97b, BNZ94, BBRT94, Boe98, BFP93, BKLv95, Bro96a, Bro96b, CBT93a, Can94, Can97, CAK+96, Cas91, CV99, CA90b, CPA95, Cos96a, Cos96b, CCZ97, CDC98, Cul91, CC96, DP94, DC97, DdJN95, DZOR98, EMMS94, FT95, FDF97, FKR92, GJOV97, Gra97b, Hag94, HBL99, Ish91, JCA97, Jay92, KM92, Kar98, Ken97, Ken98, KL93a, KZ94, KKL90, KY93, KN92, KMM95, LM91, Les91, LFD94, LF90, LE92, MSS95, MB97a, MRBO96, MRB+96a, MCA92, MKM96, NONY97, NKUS97, NG96, NB97, Oku98, PCE95, PGM95, PKM93, PVLG93, PHBB94, PK94,

PLG95, RPB+97, SCA93, SB95, SRW96b, See97, SAFK97, SFG+98, SM92, SM95, Suh94, SKS98, WSW98, YJL92, ZWJP95, Bro96c, Cab96, CP99a, Dia99, FT96, FT97a, Gur99, LL99, MRB+96b]. effects [MCT99, MR97, PZTPMC99, RCB+99, TMR99, TCM99, VX99, WGP99, XKB+99, TBP99]. Efficiency [KKT97]. Efficient [BS95, CZ94b, Hag95, Hag96a, Hag96c, Hag96b, Hag98, LP97d, MFCA93, SPH98, TSS95, WWM+98, Sim99c]. Efforts [Sha95]. Eigenchannels [Fan97]. Eigenfunctions [Kru92, LP97c, Mor96a, NB93, Nuñ94a, Mar99a]. Eigenproblems [Ada99]. Eigenspectra [SB98]. Eigenstates [KÖ69, PB95a, XY98]. Eigenvalue [HA93, Löw67a, Sad97, WMP69, FKK99]. Eigenvalues [Aqu95, Egu96a, Egu96b, FK94, GW98b, KBWJ96, KP93, LL70, MS97a, Mor96a, Sie93, ST96a, Sim97, TE96, Wil67, Egu96c]. Eigenvectors [Wul94]. Eighth [Sim98]. Eighth-Order [Sim98]. Eikonal [CF93]. Einstein [MVL98]. Einstein-like [MVL98]. Elastic [Sim98]. Elastin [LKU90]. Elastomeric [LCP+91]. Electric [ABB93, ABDM94, ASM91, Bau97, CT95, Can94, CJA94, DB94b, Fer92, Gus98, HC96e, Kar98, LF90, Mar91, MKM93b, NY98, NG95, OK96, PNB94, SM94, SBAD90, SKZ96, ZZ93, KA96, Kie97, MCT99]. Electric-Field [HC96e, MKM93b, NG95]. electroactive [GJDD97]. Electrochemical [CGSP94, YUSM99]. Electrode [WR96]. Electrodeposition [SLTMR94]. Electrodes [KPM+90, LLZ98]. Electrodynamics [KH95, RW99, Woo99]. Electroluminescent [PB97a]. Electromagnetic [CV98, OS95]. Electron [ADB95, ACHT95, AM98a, And94, Ara94, BMA93, BF96, Bad95, BK96, BS93, BN74, BL77, BCMÖ97, BH71, Bra75, BCY95, BGS98, CBT93a, CBT93b, Can94, Can97, CHM95a, CHM95b, CHMA95, CB96a, CB96c, Che93, CA97, CL94, Csa92, Day95, Day96, De 97, Del96, DP97, DdJN95, DÖ94, DZO97, DZOR98, Flo97a, FS93b, Fri93a, Fue98, FUI97, Gal72a, GVB96a, GVB96b, Hag99a, Hed95, HSES94, Ish96, IP94, JCA97, JMD95, JJ97, JM94, Jur97g, KM92, KPR97, KNN96a, KBA96, KKL90, KS96, KTCN93, KÖ69, KD95, KCP90, KCLI95, KSK91, KV96, LBBK91, LB93, LM91, LO90, LBLKC98, Löw95a, LBG97, LS92b, MM91, MSS95, MMA+92, Mar92, Mar94b, Mar94d, Mar94c, Mar96, Mar98b, MKDL93, MHS95, MB98, MM94, MB93, MBA97, MRL99, MCM98]. Electron [Mik94, MK99, MP93, MFCA93, Muk96, NNYY96, NNY+96b, NMM97, NKUS97, Nes94, NMKP94, Núñ96, Oht98, Ols96, OHSF97, Ort91, Ort92, Ort93, Ort95, Ort98b, Pai91, PGM95, Pic92, PV97, PV98, PZWJC96, PTC94, Pon97, Pon98, Pos91, PBR96b, PBR96a, RPKM95, RB93, RML97, RDK97, Roś96, RMF90, SS99a, SA96, SAR96, SSO+97, SF95a, SD96a, SN98, SG93, STMR97, SR96, Spe72a, SH90b, SM95, SW97, Suh93, Suh94, Suk95, SB92,

Csa92, FDF97, FDAC90, FADC91, GR96a, GRBA92, GRB+93, GBRA94, GNF90, GGSA98, GL95, Gör98, GMZ73, GVB96a, GVB96b, GvLB96, GVB97, GY95, HH97, HM97b, KLLB98, KCLI95, KCI98, KO95, Lah92, LP94, LG95a, LBKLC98, LR94, LG69, MS93b, Nag95b, PP98b, PS94b, PRVS95, QS98, SKN95a, SKN95b, San97, SS91, SS92c, SW71, Sla71, SS95, SS97b, Sv95, YOTY93, vBN95, FWS97, GVB96c, LCB98, SS99a]. Exchange-[Csa91]. Exchange-Correlation
[Bec94, BP95, CGLP96, GGSA98, GVB96a, GVB96b, GVB97, HM97b, KCLI95, PP98b, SS91, GVB96c, LCB98].
Exchange-Coupled [YOTY93]. Exchange-Energy
[Csa90a, Csa92, LBKLC98]. Exchange-like [CFMA95].
exchange-only [SS99a]. Exciplex [MTTS93]. Excitation
[CS98, DlD99, DP93, DM96, DTM96, DMFR93, IHG95, JY94, LD94, LD95, OJB77, Oht98, ST93, SDG97, Wen98, YLD97, DS99, LHNK99, LP99]. Excitations
[Ada91a, GS97a, MVL96, SF94, WB93, ZM95, GZDZ97, STM96b].
Excited [BLB95, BČ96b, CLSI94, CCS98, CGLP96, CC91, DD97a, Dau94, DDC97, FSBS+95, IHG95, Kan93, MLB92, MHG95, MB98, MDM94, Nag95a, Nag98a, Nag98b, Nic96, OGK90, PCN93, PTP95, RSD97, SE93a, SE95a, SC98a, SE95b, SKRK90, SGB98, Sza95, TG95, The97, TC98b, TCM98, VZ93, WS95, WD97, BGS99, MLL99, MSS99b, NNH98, SKC99, TGS99, VX99]. Excited-State
[CGLP96, DDC97, MLB92, SE95b, CCS98, SKC99]. Exciton
[ÅGL97, DP93, DM96, RM99, DS99]. Exciton-Depleting [DP93].
Exclude [GRT96]. Excluded [Art94b]. Excluded-Volume [Art94b].
Exclusion [SB92]. Existence
[AFTM95a, AFTM95b, AFO+97, AFTM98, AFZ+99]. exo
[SLG+96]. exo/endo} [SLG+96]. Expanded [GM94, PP98b].
Expanding [PCCO94]. Expansion [BF94, DLV95, GLMP98, Ish92, JM93b, Kut94, Le 97, MJS93, NS95b, Pan95, PB95c, SS91, SS92c, SP94, Sv95, TBČP95, TH90, TZ97b, TM93, VFBP96a, VFBP96b, WBD97, Hol98, LP97d, Pri98, SPS96a, VFBP96c]. Expansions
[BK94b, CB93a, DM93, HM95, JE90, Jon94, KZ99, KMP94, KMP97, KF98, MZM94, McD97, MS93b, MTL97, PR97, Sch95b, BBMM99].
Expectation [KS98, NS93b, Nuñ95a]. Experiment [BMG+98, RTKP95, SSK+92, SB97b, Sem94, GS97b, MA99a, TGDS97].
Experimental
[BKWL97, BHB+95, HH92, Jur96b, LHL91, SBM97, SS97a].
Experimentalist [WBKL70]. Experiments
[HZ93, Mar98a, Mon94, Brä98b, TD99]. explain [Bha99].
Explanation [vS95]. Explicit
[CVP90, LBPL97, LBLKC98, Kin99, Sim99c]. Explicitly
[GKKA97, JM93b, JBS97, KM99b, KA95b, Ryc94]. Exploiting

CGRB94, CA97, Csa90a, Csa90b, Dau94, DPPM94, DZ94, DD98b, DZ96a, DA91, Dob98, DDC97, Dun96, Dun97, EDH+92, Eng95, EMMS94, EMMS97, FP94, FT97b, FWC+93, Fue94, GMS97, GR94, GG97a, Gho94, GD94, GSD97, GD96, GJPF92, GNF90, Gör98, GPD94, GG97b, Gre94, GWCT97, GLBM96, GK91, HMGP93, HCR94, Hag97, HK95a, HLJ96a, HLJ96c, HHKM95, HM95, HBH98, Iva96a, Iva96b, JBT+95, JH90, Jou97, JZ95a, JZ95b, JM96c, Jur96a, Jur96b, Jur97a, Jur97b, Jur97c, Jur97e, Jur97d, Jur97f, Jur97g, Jur98a]. Functional [KD98, KS94b, KVS98, Koh95, KH96b, KL97c, LLC+94, Lev97, LLZ98, LKLBP98, LBLKC98, Lu99, LLBM+95, LAS+95, Mar95b, Mar95a, MK97a, Mar98a, MRT97, MO98, MFP96, MFAT98, MDJ98, Min90, MCA95, MNC95, MSCP92, Nag94, Nag98a, NV97b, OGK90, OHSF97, PWL95, PCE95, PP98a, Per98, PB96, PEBS97, PG96b, PG96c, PGS97, PSCZ97, PAAM98, PS94b, PSS97, RL95, RB95, RVP92, RHC96, RPB+97, RDY95, RP98a, RSD97, RRS97, SPH98, SH90a, SPOAS97, San97, SSO+97, SD97, Sch95a, SZL95, SZ96, SZ97a, Scu95, SCP91, SP92, SCP93, SPT96, SPSZ96, SPSMZ96, STY+98, STMR97, SCS94, SS91, SFM94, SAL+94, SG96a, SG96b, SG97, vH96b, Spr93, SDG97, SATP94, Suk94, Suk95, TKNI96, Tac96, TC98a, Tet93, TP90, The94, TG95, The97, TSPKM94]. Functional [TB95, Wlo95, WR96, YNY99, Yor95, ZC96a, ZC96b, ZY94, Zie96a, Zie96b, ZC95, Ali99, BDPS97, BYE+97, CCS98, CP99b, CMA+99, CEM+96, Cze99, FEE+98, GWB97, HLJ96b, Iva96c, Iva97, Jur99d, Jur99c, KK99a, KWZ98, KC97, KPB99, LBL98, MG97, MM99a, Mar99a, MVS97, MECE97, MSMR99, MLL99, MR97, PMDM97, PZDM97, PMDM98, PZDM98, PG96a, PS99b, SPM+96, SNNY99, SG96c, SC99, SNH99, TNSM99, TC98c, TGDS97, VVO98, WW97, WI98, WGP99, WMZ98, YNNR97, ZC96c, ZTC97, Zie96c, ZPBC97, Van96]. Functional-Based [JBT+95]. functional-group [MM99a]. Functionals [ABR95, ADM98, Csa90a, Csa91, Csa92, FMPJ94, Fer91, FS93a, FS94, FS95b, GR96a, GRBA92, GRB+93, GBRA94, KCLI95, LP94, LBKLC98, MPJ97, MPJ98, Per93, PV98, PRVS95, RRS97, SDW+98, SKN95a, SKN95b, SF95a, Sem94, Val94, VB94, GSKC99, MSMR99]. Functions [AS93, AL98, And94, AM98b, BDT96, BR94, CM96a, CWZ98a, CC98, Ced90, CJH98, CPTR96, CTG97, DTS97, DKWM97, DKM97, DS92, FK94, Fer95, FFD98, Flo97a, FS93b, FS97, Gal72b, GM94, GT93, Gra97a, Gui98, GOAY98, Har90, HS91, HS92d, HS92c, Hoo94, IP93, Jai70, JEB92, KSG93, Kin96, KKJ94, KT95, KRZ91, KA95b, Kut94, LB98, LDP93, LL67, Maz98, Mic96b, MCM98, Moi97, MPSLB91, MV99, NE95, Nuñ95a, Nuñ95b, Núñ97, Oht98, OK96, Par92, PVLG93, Pen93, Pen96, RC92a, RH95a, RH96a, RP96, Ryc94, SPH98, SKRK90, SH90b,

GL96b, GY95, Her97, Jur98a, Jur99d, MLT+96, RK91]. Hybridization [KN99b, KMM95, MK99, MKM96, MKM97, MM98, KN99a, KKM99]. Hybrids [HR97, Lin97, RH95b]. Hydrated [BSHP97, KRZ91, MFP96, OSS95]. Hydration [DKTZ94, PHBB94, RWT91, SD97, SSMK93]. Hydride [BFV+93, CAK+96, CPN91, SFG+98, BK97, FNSV99]. Hydride-Transfer [CAK+96]. Hydrides [BA97a, BMP93, DHLS94, DZ96b, KJ93, PZ95, PK77, PLG95]. hydrido [Gal98]. Hydrocarbon [Che93, EMMS94, KGS93, LE92, RA91, Sak98, RG99]. Hydrocarbons [DHDP92, GRK96, HA93, HGP+92, HZ94, LFD94, Luk92, ML97, Mon98, Mor97b, MBP91, RL94, Ran97, SPSZ96, SPSMZ96, SF96, BTKVG99, Dia99, GX98, Gut99a, MAC96, SPM+96]. hydrochloric [TFR99]. Hydrodynamics [MKM93a]. Hydrogen [Aqu95, AK97, BA97b, BP96c, Brä68, BCS96, CCC+95b, CCB+97, CBSR+98, CDD+99, CMFA93, CAÖ96, CR93, CLKMTA95, Cul91, DTS97, Del92, DC95, DS93, DSW93, FF94a, FT95, FT96, FT97a, Fer92, Flo95, FWBT94, FDAC90, FLF96, GBS93a, Jur97a, Jur98b, Kar90, KS94a, KS94b, KY93, KH97, Kry98, LKMC93, LJS94, MKDL93, MMRSN92, MvPC+96, Mor96a, MTD96, MPJ98, Pan93, PLA98, PTC94, PB97b, RL95, Ram90, RC92a, Ram94, RGT95, SM98, SY91, SSP98, SC94, SG98, SS92b, Suh94, SFGW96, TNM98, Taş97, TKSH93, The94, TT98, VBV92, VBUS99, WSTB90, YNMT98, ZW96a, ZW96b, AZ99, CSH99, Cor97, GT97, Jur99d, MSS99b, PZTPMC99, RFG99, SLG+96, TG96, WG99, WBS99, ZW96c]. Hydrogen-Bond [SY91]. Hydrogen-Bonded [AK97, BA97b, Cul91, Kar90, KS94a, KS94b, Kry98, VBV92, RFG99, WG99, WBS99]. Hydrogen-Bonding [FT95, FT96, FT97a, KH97]. Hydrogen-like [Taş97]. Hydrogen-Substituted [RL95]. Hydrogen-Transfer [BCS96]. Hydrogen-Type [DTS97]. hydrogenase [PBS99]. hydrogenases [GFGB99]. Hydrogenated [AST93, HU94, KI94]. Hydrogenation [SWMB94, SZ98]. Hydrolases [HBH98]. Hydrolysis [HBH98, PHBB92, STS95, TSS95, WP92, WJC+98]. Hydrolytic [PHBB95]. Hydrophobic [AV92, NK96a, PB97b, Urr94]. Hydroxides [BK94c]. Hydroxo [CdBKZ99]. Hydroxo- [CdBKZ99]. Hydroxy [MRT97]. hydroxyketones [FWZ97]. Hydroxyl [BHPB93]. Hydroxylanion [JPD67]. hydroxylation [SRP+98]. Hydroxylations [CD90]. Hydroxypentanoic [Flo95]. Hydroxypropanal [OSA+97]. Hydroxypropionic [CFR96]. Hydroxypyridine [MTD93]. Hydroxytetronic [BKEMM94]. Hydroxyurea [LB96a]. Hylleraas [BKL98, FR98, KL93c, HMLK98, KBL95, PCCO94, US96]. Hylleraas-CI [BKL98, KL93c, HMLK98, KBL95]. Hyper [JCA97, LS71]. Hyper-Hartree [LS71]. Hyperboloidal [LKMC93].

MGLBP95, MFCA93, Ort95, PMN+92, PCCO94, SPH98, SBD+92, SH90b, TNI96a, TNI96b, Thu75, TL79, US97, US96, WL67, ZZ93, CM99, DD97b, Jon93, Kin99, MRC99, Smi99, TNI96c]. Integrand [FS94, FS95b]. Integrated [CDDV93, KKK90, KK91, KM97, MSM96, MK95, MK96a, MK96b, MK97b, MK96c]. Integration [Csa92, FS93a, IYFI99, Roc99]. Integrations [JE90]. Intelligent [JCM+92]. Intense
[BRZY97, CFB97, DlD99, DD98a, Mar91, Mar92, NY98]. intensities [MSS99b]. Intensity
[DMR96a, DMR96c, DMR96b, GDID98, McH91, MLK94]. Interacting [CBG94, GJOV97, Mar93b, MR99, Nak92, GT97]. Interaction
[Ada96a, Ada96b, Art94b, BHL+99, Bat92, BE93, BEG94, BP96c, BHV96a, BHV96c, BLG95, BL98, CPBC95, CCC+95b, CCB+97, CLR+93, CF96, DS96, DDG93, DFL98, DS93, Duc90, DM94, ESP98, EBG95, GS68, GRT96, GVB96a, GVB96b, HP98, Huz96, Ish91, IHG95, JKK+92, JTZ+96, KSR95, KBKT93, KRZ91, KKE+96, LB94, MMRSN92, MALT96, MC97a, MHG95, MH68, MR92, NTL96, NI94, Pai91, PS96, Pec93, PAC98, PFMC97, PS68, Pro94, Pro95, SWF93, SM96b, Sas74, SF95a, Sch99b, SCS94, Sur94, Sur95, SJR91, TL79, TMDB98, VA90, WP90, WMW92, YZX96a, YZX96b, YDDP92, YJL92, Yu95, ZC91, Ada96c, BHV96b, CGG96, CDP+99, GVB96c, ISOA99, LLB99, MMCC99, MLT98, Men99, NL96b, SWD+99, SEKEB98, TSY99, TC98c, YZX96c]. Interactions [Ada90, Ada91b, And90, BP93b, BP93a, BMP92, CMSF93, DE92, GBVM93, Gin97, KSN95, Kar98, KPTS+93, LV93, LS93a, Man95, May92, May98, MK90, NNMH96, OB95, OLC+96, PWL95, SE93b, SD98, SGB97, vH96b, SPL97, TWK+92, ZRNZ97, AGM99, CG97b, CPGC99, HVS98, JMP99, KPTVT+97, KH97, Man99, MVHV96, RMH+99]. Interatomic [RA96]. Interband [SMM+90]. Interbasis [KMP94, KMP97]. Interbond [Sur95]. Intercalated [Sta98c, vS95]. Intercalates [BLC95]. Intercalators [HGP91]. Interconversion [TCB99]. Interconversions [BHPB95, HRH99]. Intercorrelation [HGP+92]. Interelectronic [GR95b, GR96b, Lah92]. Interface [CCT98, Kov98a]. interfaces [WGP99]. Interference [May92, SS96]. Intergration [JO94]. Interim [Har97a]. Interionic [Mez94a]. Intermediate [CPN91, EZ92, NMN+97, NMN+98, Pai97, PL98, SS99b, ZM95, BHGC99, FF96, Pai99]. Intermediates
[BP92, EMMK94, HS95, HDB+95]. intermetallic [MECE97]. Intermolecular [Ada90, Ada91b, Ada96a, Ada96c, Ada96b, Ada99, BMP92, EE91, GBVM93, KBKT93, May98, McH91, Pie93, Sco90, SPL97, SJR91, TT98, VH96a, HVS98, JMP99, MVHV96]. Internal [BW99, Che97, GWCT97, KC98a, KLC98a, KC98b, Pal97b, Sch92, ZZCSE94, CLZ99, GX98, MJLL99]. International [MDS98].

[ABB93, ANB96, Bar90, KA96]. Metathesis [SC97b]. Methacrylic [FY95]. Methane [CRSP93, CC96, Jur99b, YNMT98, BYE+97, YNST99]. Methanediol [BAK96a]. Methanes [BMP92]. Methanetetraol [BAK97]. Methanetriol [BAK96b]. Method [Ada91a, ADB96, AB97, ASI94b, Bat92, BCMÖ97, BLBP97, BD94a, BD94b, BD94c, BA90, Boe95, BR94, BS95, CMCR96, CZ94b, CS96a, CS96b, CVW91, Cul91, DE92, DM95, DM97a, DKWM97, DKM97, Duc90, Dun99, FSBS+95, Fer92, FZZ92, GGSA98, GRTR96a, GRTR96c, GH96a, GMI95, GG97b, GB90, GLBM96, Hag96a, Hag96b, Hag98, HK95b, Huz96, IK94, Iga95, IANK94, Ish92, JM95, JGR98, JMR98, Kal90, KUN+98, KBGE97, KNN96b, KNN96d, KKNN97, KPA95, KSY97, KF96a, KF96b, KY93, KLLI97, Kry95, KB92, LO93, LVL+93, LS71, LK90, LH94, LL67, LJS94, Löw68b, MHS95, MV98b, MSM96, MB98, MB93, MS97b, MBA97, Mik94, MAD98, MAI95, MAI97, MAPLB92, NNYY96, NNY+96b, NKSN96, NKS+96b, NONY97, Nag96a, Nag96b, Nag98b, NSTFC94, Nes94, NS93a]. Method [PIG94, PSAUS90, Pau92, Pec93, Pen93, Pen96, PCCO94, PDT97, RDF98, RL95, RRC94, Réc90, Rin96a, Rin96b, RL97, RL92, SWF93, SPOAS97, SZL95, SS99b, Sim98, Sin92, SBD+92, STM96a, SDG97, TMSI98, TR94, US96, VJ95, VJ97, WMP69, WTS97, WDD93, YD97, YITY93, ZM95, ZLHZ94, Zho93, ZWJP95, Zou92, AS99, BRV99, CS96c, DKM96, FNSV99, GHB+99, GRTR96b, Hag96c, HZ99, HK97, JM96a, hJH97, KNN96c, KF96c, LKM99, LP97d, LP98, MRC99, MHY98, MR97, NNY+96a, NKS+96a, Nag96c, New97, RAI99, Rin96c, Roc99, vG96, SWD+99, STM96b, TSY99, Tho96, Tit96]. Methode [JPD67]. Methodological [GNA98]. Methodology [BPL97b, Del92]. Methods [ASP97, ANB94, ACAT92, BBSS96b, BBSS96a, BIM97, BLE96, BBS+97, BLRD92, BF94, BL92, CCM+96, CZ93, DS90, DSS90, DRBE96, DZO97, DKBB97, GD96, GL92, GMZ73, Hag92, Hag95, HS92a, HK95a, Her98, HSES94, HS91, HS92c, Jak93, JO94, JK92, Jug96, JM96c, Jur97a, Jur97b, Jur97e, Jur97d, Jur97g, LZ92, Löw99, LS92b, Mar95c, Nic99, PMN+92, PTH+97, RL94, RHC96, RWT91, RC92b, RWT92, Roz97, SAW97, Sch95c, SRM98, Sim95, Sim97, SES93, SAL+94, SG96a, SG96b, SG97, SGB97, SGB98, Sta93, SATP94, Sza95, UWB94, VFHL93, WL67, WR96, YBZ92, ZON+96, ZZZY96, BBTU97, CMA+99, Gut99b, HC96c, Jør92, KK99a, KLO+98, MG97, SGGC99, Sim99c, SG96c, WGP99, BBSS96c]. Methoxy [HS99]. Methoxyidazoxan [HS92a]. Methyl [HDY+91, MZ93, NSS+95, PVF+92, PSCZ97, STS95, vS95, MJLL99, RT99, SCJK90, SSM+99]. Methyl-Ethyl- [NSS+95]. Methylacetamide [TT98]. Methylamine [AMKS93]. Methylated

Zha92, dVJ93, BPHB96c]. model [CVP90, CF99, GWB97, GJDD97, GL96c, JM96a, KF96c, MUL99, MMCC99, MRB+96b, MCT99, PZTPMC99, RC99, TD99, TCM99, TNS96c, Vin92, WDS97, YNST99, YNNR97]. Model-Systems [Sch99b]. Modeled [Csa92, CPGC99]. Modeling [ADB96, BHV96a, BHV96c, BS95, CAK+96, CL95, DAF+96, DS92, DSW93, GJ95, GRTR96a, GRTR96c, GX95, Jen94, KE91, Kun90, LV93, MLT+96, MCB99, NTL96, NG97, RMH+99, SD97, SKZ96, SM92, TBP99, TSS95, YDDP92, vS95, AFM99, Bla99, BHV96b, GRTR96b, KÅ99]. Modelling [SKJ98]. Models [ÁC94, BXZ95, BHX96, BMK96, Bra96, CAÖ96, CL92, Eri93, Fer91, FP96, HDB+95, JG95, KD98, LV93, MLA93, MALT96, PFMC97, PTH+97, REL+90, SG94, STZ96a, STZ96b, Tch96b, Tch96a, Yam97, BRS96, GFGB99, MCB99, OCK99, SAB+97, SRP+98, Sim99a, Sim99b, STZ96c]. Modern [Amo96, CTG97, KGC+96, Kla93, Löw97b, Oli99, SPT96, TC98b, Kry96]. Modes [HW91, KC98a, KC98b, PP98b, WD91, JDB99, KLC98b]. Modification [Bee79, GRT96, GRTR96a, GRTR96b, GRTR96c, Iva96a, Iva96b, Iva96c, Iva97]. Modifications [Sta98a, WZW96]. Modified [BE95, Fue98, MMP95, MK99, Pec93, Por99, RL92, SWMB94, Taş97, ZARB96, BGS97, Hol98]. modified-Hartree [Hol98]. Modifying [ZZZY96, ISOA99]. MODPOT [PK76, PK77]. MODPOT/VRDO [PK76, PK77]. Molecular [AEAO99, AHM97, ARDP92, ACAT92, AP96, ÁC94, ATI97, AM98b, AM90, Art93, Art96a, Art96c, Art96b, Art98, Ata94, BBSS96b, BBSS96a, BKR97, BC96a, BL77, BSB94, BM96, BCMÖ97, BLBP97, BSHP97, BG98a, BBLK94, BR94, BFH96, BH71, BMP93, BVV91, BMVV93, CCM+96, CMCR96, CFB97, CC97a, Cio94, CG96, Con92, CA90b, Coo94, CE90, DE92, DP93, DM96, DTM96, DN96, DAF+96, DZF93, DÖ94, DO90, Dun98, ESHP99, Eld73, Enk97, ECBH96, Fan97, FWT+96, GBVM93, GVK99, GJ95, Gho95, GRT96, Gin99, GT93, GPD94, GG97b, GMZ73, GGHP94, GLBM96, GW98a, Gus98, GLLY94, HAEMA92, HS92a, HGC93, HL93a, Her97, HSWS95, HDB+95, IYFI99, JO94, JM96b, JE90, Jon94, Jos97, KUN+98, KFS92, KPD93, KP75, Ken97, Ken98, KKK90, KK91, KK92]. Molecular [Kin93, Kin94, KM97, KN99b, KE91, Krü97, KPB99, KL92, KL97c, LB96a, LJ95, LZ96, LP97b, LLC+94, LYSL95, LHL91, Les92, LDP93, Lip91a, Lip91b, Löw99, LL92, LKU90, LCP+91, LBG95, Mar90, Mar94d, Mar95a, MHÅ98, MKM93a, Mar95c, MC97b, Mat99, MM94, MR99, MCA92, Mez94b, Mic97, MLK94, MK99, MAI95, MH98, MSCS95, MK95, MK96a, MK96b, MK97b, MK98a, MK98b, Mor97a, MV99, MSCP92, MAAP+98, NKSN96, NKS+96b, NK96a, NY98, dMNZdA92, NP96b, OMTS97, ÖOD96, OSA+97,

Pen93, Pen96, PVU$^+$93, Pic92, PC95, PAAM98, PJ96, PK76, PK77, RTKP95, RKN97, RK97, RD98, RFM90, RWT91, RWT92, RW98, Roś96, RK91, RCWN94, RAM91, RMF90, SM98, SCA93, SM96b, SHF94, Sch95a, Sch95b, Sch95c, SC96a, SC96c, SNMB97, SCP91, SCP95b, SS99b, SRS92]. Molecular [SCJK90, SG94, STMR97, Sla67a, Sla71, SGGMGFS96, SKRK90, SMO$^+$96, SM92, vH96b, Ste96, SP94, Sul97, Suz99, TMSI98, TH90, Tal93, TMP97, TD96a, TW90, The94, TPM70, Tho96, TC98b, Tom91, TNM97, TD96b, Tul91, US97, US96, UBA92, UWB94, VBV92, VFHL93, WS94a, WLBL94, Wan94, WP90, Wil96, WGRM94, WP92, Wul94, YTYS97, Zha92, ZLHZ94, ZM96, ZM97, BBSS96c, CM99, DS99, FMD$^+$96, GJDD97, HOF$^+$97, KH96a, KKNY99, KWZ98, KÅ99, Kry96, KSW98, KSK$^+$99, KKM99, LK99, Lei99, LF99, LV97, MLL99, MK96c, MPIP99, NKS$^+$96a, NMN$^+$99, NYNY99, NL96a, NL96b, OKY$^+$99, RC99, SX96, SC96b, SGGC99, SOK$^+$98, TTM99, TCB99, VES$^+$99, WW97, WGP99, Woo99, Brä98b, KN99a, SK99a]. molecular-state [KSW98, KSK$^+$99]. Molecule [AS96, BBC$^+$94, Brä68, BvL96, CWX93, CRSP93, CCC$^+$95b, CCB$^+$97, DB99, Del96, GSM90, Gin98, GS93, GYDY97, HBL99, JCÁ96, KM92, Kon94, KA95a, LLL92, LD95, MMRSN92, MHM95a, MB98, Mon99c, MTD96, MPJ98, Nak92, OTS$^+$95, OJB77, PGM95, PVLG93, PLA98, Pie93, PTC94, Ran93, RGT95, SG93, dSdSN95, SZ98, TKNI96, TMSI98, VLCBPR97a, YTYS97, BSS$^+$97b, CWJ$^+$99, GJPZ97, HGL99, Ike99, MUMH97, NWG$^+$99, SOK$^+$98, TGS99, TG96]. Molecule-Surface [GYDY97]. Molecules [AHI96, AZAC97, BBOR96, BJMT94, BK95, BKM93, BEJ98, Bro95, BZQ95, BLG95, BK98, CT96, CAK$^+$96, CC95, Che97, CBL95, CTC95, CL94, DTA$^+$96, DlD99, DDH$^+$96, DKWM97, DKM97, DA91, DT96a, DT96b, FLHT90, FCVL98, FSF96, GS92, GSPSM93, GG97a, Gra97a, Har96, HP97, HS95, Hil98, HHHP99, ILL96, IP93, Jai70, JY94, Joh67, JOC97, JCM$^+$92, JAG95, JM96c, Kan93, KVB97, KP75, KM90, KPTS$^+$93, KT95, KD95, Kru92, KMM95, Kup98, LDGA96, LKMCVT95, LKMCVT96, LTP96, LN96, LSC98, Mar93b, Mar94b, Mar98b, MKDL93, MHG95, MRL99, MW90, Min90, MR92, MKM96, MKM97, MLT$^+$96, Mor93a, MP93, MIW91, MSPS90, Nes71, NE95, NK98, Pal97b, PP98a, PBB94a, PWC96, PPK97, PK94, RPJZW96, RD98, RF94, RL98, RD90, RABZ94, Roś96, RS97a, Ryc94]. Molecules [SC91, SC97a, Sch98, SD96a, Sco90, SPF96, Shu96, Sin92, SSM90, SKRK90, Sta96a, Su93, Suk95, Suz99, TNSE94, TFSZ95, TKK$^+$90, TDO97, VdV96, VA90, VHFL93, WP93, WS95, Was96, WZW96, WHPC95, WMW92, YDFS98, ZA95, ZWJP95, ZZCSE94, AI99, BKY99, CCWCF96, CXFP99, CS99, DKM96, Deu98a, DT96c, GL99, GDYY97, hJH97, Kov98b, LCS98, MSMR99, MKBP97,

BFV94, DlD99, JY94, KSK91, Moi97, Ata97a, Hag99b, LA97]. Multiple [AT99, And93a, BC97a, GR95b, GR96b, GH96a, HGC93, JM93a, JKJ94, JKJ95, Joh67, JSG97, MKM97, MBML91, SBLL94, SKRK90, SLL$^+$91, YPC97, TC98c]. Multiple-Reference [GR95b, GR96b]. Multiple-Transient-Point [And93a]. Multiplet [PG96b, PG96c, PG96a]. Multiplets [KT96, Nag95b]. Multiplication [KL93b, FCMB99]. multiplicities [STM96b]. Multiply [BCLS94]. Multipolar [BP96b, LS93a]. Multipole [Gus98, KY93, KJ93, Le 97, McD97, Pan95, PNB94, ZZ93, SPS96a]. Multipoles [ÁC94]. Multiquantum [Kov98b]. Multireference [vDvLR99, DM94, Hir92, JG95, KD95, WSW96a, WSW96c, WSW96b, Wen98, Cim96, MUMH97, TGS99]. multishell [BG98b, BG98c, BG98d]. Muon [SJ91]. Mushrooms [Art97]. Mustard [BHV96a, BHV96c, BHV96b]. Mutagenic [PWL95]. Mutation [LF90]. mutations [NWG$^+$99]. Mutual [GJ95]. Mutually [Bro93, DMFR93]. My [Roo93a]. Myb [JTZ$^+$96]. mylar [Por97]. Myoglobin [SPC96]. Mystery [SS96].

N [CEM$^+$96, SSM$^+$99, WYW96, YK97, ZC96a, ZC96c, ZC96b, IP93, AEAO99, ABDM94, ASM91, DSS90, DZ97, Eva97, FdCC92, Gao93, GS93, Hir92, HB95, Kal90, KBGE97, LC93, MK90, MM94, MZ95, PGS97, RK95, SE93b, SK99a, SP91, SSM$^+$99, SES93, STC96, Tew94, Tew97, Bou94, Kal90]. N- [LC93]. N-Acetyl-2 [RK95]. N-Sulfinylanilines [AEAO99]. N-threonylcarbonyl [SSM$^+$99]. N. [Kum93b]. Na/W [KO95]. NaBr [MTNF99]. NaCl [JMD95, JSG97]. NADP [GVK99]. NaK [Man99]. Naked [HCR94]. NaN [YK97]. Nanometer [KDHW90]. Nanoparticles [ZLWES99]. Nanotubes [TAY$^+$97]. naphthalene [VLCBPR97b]. naphthalenophane [RGHH94]. naphthalenophane-1 [RGHH94]. Narrow [Ara94]. Narrow-Band [Ara94]. native [TD99]. Natta [Sak97]. Natural [BW99, BCD95, BC93, Cio90, LO90, Löw95b, Löw97b, PKM94, WZ94]. Nature [Bad95, DP94, Fuk95, Kap99, Löw67b, SG93, SLL$^+$91, CP99b]. NB [JMP99, SAB$^+$97]. NBMO [AI99]. Nd [Bou96c, Li93, Bou96a, Bou96b]. NDDO [NSTFC94, Ney95a, Ney95b, Cul95, SGGC99, FZZ92]. NDDO-based [SGGC99]. NDDO/MC [FZZ92]. Ne-Isoelectronic [SS92a]. Near [Bad95, Dat95, GSSD$^+$96, Kov98a, MVL96]. Near-Infrared [GSSD$^+$96]. Near-Sighted [Bad95]. nearly [vMVvLvD97]. Need [RWT91]. Negative [BJLK98, Sie93, ZW96a, ZW96c, ZW96b]. Negative-Energy [BJLK98]. Negatively [HL93b, NS97a]. Neglect [EZ92, NSTFC94, NS95a, NS95b, NE95, Ney95a, Ney95b]. NeH [PHH94]. Neighboring [Gin97, SY91]. Neocarzinostatin [MC94].

FDD95, NS95a, NS95b, NE95, Ney95a, Ney95b, ROL+90]. Nonequilibrium [CT95, GG97a, KH90, RB95]. Noninteger [KKT97]. Nonintegrable [Pri95]. Noninteracting [HM95]. Noniterative [NU95]. Nonlinear [ADB95, Áng93, CV98, CT96, DB94a, Hom93, Kie97, LO93, LFS94, Mar93a, Mor93a, Ott94, PB95c, PB99, PK94, SPH98, SM99, SB97a, Sch93, Sch94, Wen96b, Wen96a, AMC97, PFK99]. Nonlocal [ABR95, AS95, CGRB94, CA97, EMMS94, FT97b, FSVZ97, GRBA92, GBRA94, RRS97, Sem94, VB94]. nonlocality [MA99a]. Nonmetallic [RMPR98]. Nonorthogonal [DV98, Fer96, Iga95, CB99]. Nonorthogonality [Sin92]. Nonparabolicity [EC96b, EC96c]. Nonperfect [CR96b]. Nonperiodic [MAI95]. nonplanarity [HGL99]. nonproduct [DD97b]. nonradiative [BKY99]. Nonrelativistic [AH97, BKL97, BLK97, BKL98, GLMP98, HMLK98, RW99]. Nonresonant [CPA98]. Nonrigid [BK98, Kel97, SSM90]. nonrigidity [HGL99]. Nonseparable [TE96]. Nonsingular [BSS97a]. Nonspherical [LB96b, LB96d, LB96c]. Nonstandard [JM96a]. Nonstationary [NMKP94]. Nonsteroidal [dAdM95]. Nonuniform [Iva96a, Iva96b, Iva96c, Iva97]. Nonunitary [BA93]. nonzero [BG98c]. norbornenone [KH96a]. Normal [DJ95, HW91, KC98b, NK98, PP98b, KLC98b]. Normal-Mode [DJ95]. Note [Bee72, BDT96, BNLF96, CC97b, DC95, Sla70a, TMH94, Wen93, AB99]. Novel [DBG92, DQB97, EK94, SP94]. novo [SKM99]. NR [PZTPMC99]. NSF [FG96]. Nuclear [AS96, AO93, BCMÖ97, DÖ94, GSM90, GR95a, HS91, JBT+95, Mic96b, PTC94, RGO94, SPH98, US97, BCC99, Bla99, FV96, Hag99a, KH96a, MTNF99, SK99b]. Nuclei [ASM91, VCCM92]. Nuclei-Centered [VCCM92]. Nucleic [AP96, Les92, RFG99, Tew94, SSM+99, Tew97]. Nucleophiles [PBB92]. Nucleophilic [DD93]. Nucleotide [LJS94, YJL92]. Nucleotides [KJL96b, KJL96a, KJL96c]. Number [JM96b, TT98, TMH94]. Numbers [HS92b, KKT97, KS96, KTCN93]. Numerical [AHI96, AH97, Bra97a, CGSP94, CFB97, Csa92, Csa96, DP93, FDF97, FS93a, GPD94, GMZ73, GWCT97, Hag95, Hag96a, Hag96b, Hag98, IYFI99, JE90, KWT95, KT95, Loh96, NY98, NYNY99, Nun94b, Roc99, SB95, SB97b, Tal93, Thu75, WL67, Hag96c, SN99]. Numerov [Sim97]. Numerov-Type [Sim97]. NWChem [BAF+95].

O [BILA95, BDH+97, CLOFR98, IBS95, Jur97e, Li93, LF95, MGNK95, MZ95, NM95, Ort98b, RCWN94, SRP+98, TJ97, WI96c, WI96b, WL99, WMD95, XYC98, ZBL99, ABDM94, BA91, BYE+97, BYGA99, CGG96, CB93b, CB94a, Csa96, DSS90,

PMS94, RW92, Spr96, TFSZ95, TZCT97, XSG97, BL99, BGS99, BT96b, Dia99, FMD+96, Fra99, GJDD97, KP96, Li97, MECE97, PS99a, SZCO99, TST+99, WG99, BHGC99, KJ97]. Students [Ano99n]. Studied [FWT+96, LSGS91, PIG94, RHC96, Ryd94, SAFK97, TNSE94, ZY94, GZSvD99, hJH97]. Studies [ART94a, dAdM95, AK97, BKWL97, BJMT94, BHH92, BZQ95, BCS96, BDH+97, Cai93, CL97, CCC+95a, CPBC95, CBSR+98, CXL97, CDC98, EZ92, FF94a, FF94b, FT95, FB96, FLF96, GBVM93, GJLA99, GL96a, GL96b, HCR94, Har97a, HS92a, HHKM95, HBH98, JY94, Jur98b, KSR95, Kar90, KS94b, KN92, KL92, LKM99, LYSL95, LSS96a, LSS96b, Les92, LX95, LB94, LC93, Löw68b, LG71, LKU90, LCP+91, MZ95, MR92, MZ93, MGK99, MC95, Mor98a, MFCA93, NNMH96, NONY97, Nak92, NHN97, Pau92, PVLG93, PBB94a, PS68, PCF94, PS94b, RKPE95, RKG96, Sak97, SA96, SP92, SCP93, SSM90, Spr93, Sta98a, SZ98, TZCT97, TCZ91, TSPK96, TB95, TD96b, WY95, WP92, YOTY93, YXX99, YTYS97, ZYY95, BH99, CP99b, DA97, DP96, FT96, FF96, FT97a, GFY+99, GL96c, Hag99a, HWB97b, HWB97a]. studies [LSS96c, NMN+99, NL96b, RC99, Tri98c, WJC+99]. Study [AL95, ADB95, AKD96, AP93, ANB94, AMT+99, AHI96, AR96, AMKS93, ABCM93, ADPS98, BLC95, BAR94, BA97b, BAN97, Bat92, BBOR96, BTTS97, BJ98, BILA95, BEG94, BCLS94, BLE96, BBC+96a, BSP97, BSHP97, BHX96, Boč96, BP92, BHH92, BjH97, BAK96a, BAK96b, BAK97, BCRL94, BPL97b, BRA+99, Bra97b, BHPB93, BHPB95, BVV91, BMVV93, BS95, BMG95, Bue96, BLG95, BDD93, BK94c, BvL96, CBAM97, CWX93, Cai94, CdBKZ99, CPN91, CRSP93, CCC+95b, CCB+97, Che96, Che97, CL92, CA97, CCZ97, DS96, DD97a, DN96, DDRB96, DAR+96a, DB94a, DSS90, DD96a, DD96c, DZ96a, DV91, DZ97, DD93, DDC97, Dun99, ESP98, EMMK94, ET97, ET99, EDF+98, FY95, FLRV97, FMDA94, FDF97, FGM90, FL95, FDD+93, FWBT94, FKR92, Gal96, GG97a, GD96, GBL97, GL98, HK95a, HDY+91, HP97]. Study [II94, JGCJ96a, JGCJ96c, JKK+92, Jai70, JKRW98, JGR98, JMR98, JDJP99, JMS95, JSKC95, Jur96b, Jur97f, Jur99b, Jur99a, KW92, KSN93, KI94, KH96a, Kry98, KGVM97, KG99, KL97c, LV93, LJ95, LMV92, Les91, LHL91, LGT94, LH94, Lio92, LFD94, LSC98, Lu99, LBG95, MKK96a, MKK96b, MKK98, MRT97, MCOS94, MKDL93, MMRSN92, MLA93, MALT96, MTP+98, MDD93, Mav98, MB98, MG93b, MRL99, MTD93, MDJ98, MY99, MK99, MC94, MKM96, Mor97a, MBML91, MCA95, MS90, MBP97, NSS+95, NN94, NFVM94, NM95, OTS+95, Oli99, Pal94, Pan93, PMM97, PP98a, PHH94, PFMC97, PLV92, PPP97, PM93, PBB92, PB95b, PZ95, PMJM+91, PHBB92, PBBH93, PHBB95, RL95, RTKP96a, RTKP96b, RM96, Réc90, RGHH94, RK91,

Pop98, AFZ+99]. Theoretic [Del98, Dun99, PMM97]. Theoretical [AP93, dAdM95, AMT+99, AFM99, AMKS93, ADPS98, ASI94b, BMA93, BLC95, BKWL97, BAR94, BF95, BA97a, BSB94, BSP97, BD95, BH99, BjH97, Boe91, BHGC99, BHB+95, BZQ95, BK94c, CPN91, CRSP93, CPBC95, CCC+95b, CCB+97, CBSR+98, CS96a, CS96b, CWJ+99, CS99, CSH99, CPD+98, CDP+99, CDDV93, DA97, DTA+96, DM97b, DB94a, DS90, DSS90, DD96a, DD96b, DD96c, EK94, ET97, ET99, Eng95, Eri93, ECBH96, FMS+99, FY95, FWZ97, FMDA94, FDD+93, FB96, FLF96, Gal96, Gal98, HJ94, HDY+91, HB95, HWB97b, HWB97a, II94, Jen99, JZ95a, JZ95b, KW92, KSN93, KA96, KE91, KCI98, KPM+90, KMM96, LYSL95, LHL91, LFD94, LC93, LBBE98, Löw94, LSC98, LCS98, MV98a, MKK98, Mar95c, MMRSN92, MMCC99, MALT96, MTP+98, Mav98, MRBO96, MRB+96a, MG93b, Men99]. Theoretical [MY99, MBML91, MPOG99, MC95, Mor96c, Mor98a, MS90, NONY97, NMN+99, NTL96, Nak92, NN94, NHN97, NNH98, NST94, OLC+96, Ott94, PWL95, PP98a, PMJM+91, PHBB92, PBBH93, PHBB95, RGHH94, RCWN94, RKG96, RW92, Sak98, SKTN97, SL93, SRP+98, SCA93, SWMB94, dSdSN95, SBOB97, SES93, SGB97, SGB98, STZ96a, STZ96b, TP94, TST+99, TC98a, TFSZ95, TZCT97, TCZ91, TB95, VMCK97, WY99, WJC+99, WY95, WMD95, WMZ98, XY98, XY95, YOTY93, YXX99, YDDP92, ZJS99, ZBL99, ZSK97, CS96c, GBS99, HRH99, JMP99, MRB+96b, SM96a, STZ96c, SC98b, WBS99, CMA+99, DM98, KP96, KWZ98, SPT96, Tit96, TM99]. Theoretically [FF90, YLLJ96]. Theoretically-Derived [FF90]. Theories [BG95, KS98, Lev97, NS95a, NS95b, NE95, Ney95a, Ney95b]. Theory [ÅGL97, Ada90, Ada91b, Ada96a, Ada96b, Ada96d, Ada99, ASI94a, AC95, ABR95, AR93, And94, Áng93, Aon99, AO93, BDG96, BAR94, BS75, BIM97, BX94, BG98a, BA93, Bra75, BAD99, CGR74, Cal93, CT95, CG97a, CC95, CJA94, Cha98, CGLP96, CSP98, CDDM96, CJH98, Chr97, Coh97, CA90b, CA91, CPA95, CB94b, vDvLR99, Dau94, DZ94, DD98b, DA91, DZOR98, EDH+92, EKI94, Eng95, EMMS97, EZ92, FP94, Fer92, Fri93a, GDID98, GR94, GS68, Gho94, GJPF92, Gin98, Gin99, GNF90, GL95, Gör98, GG97b, Gra97b, GWCT97, GK91, Hag97, HLJ96a, HLJ96c, HHKM95, Hir69b, HBH98, ILL96, IY99, Ish92, IYFI99, Jac92, JG95, JM93b, JPJ95, Joh67, JM96c, Jur96b, Jur97a, Jur97b, Jur97c, Jur97e, Jur97d, Jur97f, Jur97g, Jur98a, KBT94, Kar98, Kar94]. Theory [Kir95, Kla93, KZVGB97, KSY97, Koh95, KD95, KCLI95, KG99, Kum93a, Kum93b, Kut94, KL97c, LL94b, Lef99, LP96, Lin97, LL68, LD94, Löw68a, Löw68b, LG71, LZ92, Löw96b, Löw99, LLBM+95, LAS+95, LJN+98, Mar92, Mar95b, Mar95a, Mar98a,

MO98, MHM95b, MHM95a, MC97a, MC97b, Mat99, McW90, MB93, MCA92, Mon93, Mon94, MV99, NOYY94, NYY96, Nag94, Nag98a, NU95, NMKP94, NV94a, Oli99, OGK90, Ort91, Ort92, Ort93, Ort95, PL93, PV99, PP98a, PEBS97, PLA98, PM93, PG96b, PG96c, PSD97b, QS98, RDF98, RL95, RB95, RVP92, RH96b, RZ96, RPB+97, Rin94, SSK+92, SPH98, SH90a, Sah95a, SD97, SZ96, SZ97a, Sch93, Scu95, SB96, SPT96, SG98, SAFK97, SN98, SAS99, STY+98, SS91, Sla67a, Sla71, vH96b, Su93, Suh93, Suk94]. Theory [Suk95, SPL97, Sv95, SB92, SJR91, TKNI96, Tac96, TMP97, TC98a, Tet93, TG95, The97, The98, Tob99, VLCBPR97a, VVS94, VDL95, Wal94, Wan94, WB93, WL99, Wen98, WHPC95, Wlo95, WWM+98, YL94, Yor95, ZLHZ94, ZC91, ZY94, Zie96a, Zie96b, Ada96c, Ali99, BSP98, Brä98b, BDPS97, CWZ98b, CCS98, Cim96, CEM+96, Cze99, DP96, FS99, GZSvD99, Gut99a, HR99, HC96a, HC96b, HC96c, HC96d, HLJ96b, Jur99d, Jur99c, LK99, LBL98, MHN98, Mar99a, MVS97, MUMH97, Mat96, MM99b, McW99, OKY+99, Ort97, PMDM97, PZDM97, PMDM98, PZDM98, PG96a, SS99a, SOK+98, SNNY99, SC99, SO97, SNH99, TNSM99, TMA97, TC98c, TGDS97, VLCBPR97b, VVO98, WMZ98, ZC99, Zie96c, ZPBC97, LP98, Brä98b, Gre98, Jør92]. Theory-Based [BDG96]. therapeutic [WWFR99]. There [Ada90, KJ95]. Thermal [BMK96, KW92, LMR94, RW92, Tob99]. Thermochemical [Bec94, HPSC97]. Thermochemistry [GBL97]. Thermodynamic [VH96a, Chu99]. Thermodynamics [FDD95, FD96a, Mic96a]. Thermolysis [ZH99a]. Thiamin [FB96, FFN98]. Thiazole [MH98]. Thickness [Boe92, MPV94]. Thin [Bat92, Boe92, MV90, MPV94]. think [Ber96c]. Thioacetone [SSM90]. Thioanisole [DZOR98]. Thiocyanate [Pro94]. Thioformacetal [BV93]. Thioformaldehyde [GH96b, GH96c, GH96d]. Thioguanine [RBBL94]. Thiooxamides [KM90]. Thiophene [BSB94, SL98]. Thiophene- [SL98]. Third [BSB94, DM94, LFS94, NK96a, Suh93, SPL97, VFHL93, ZO95, Ort97, PWL98]. Third-Order [BSB94, LFS94, Suh93, SPL97, VFHL93, ZO95, Ort97]. Thomas [Csa92, Csa96, MK97a, MHN98]. Three [ABB93, ANB96, Art98, DM96, DTM96, GSPSM93, GBL97, HS91, Hoo94, KFS92, KJ95, PM95, PPP97, Pie93, RA91, SPH98, Sta95, Sta96a, Sta96b, Sta98d, Sta98e, VDD96, WD95, WD97, DS99, Kin99, LL99, MVHV96, Sta98b, NM96]. Three- [GBL97, PM95, PPP97]. Three-Body [KFS92, Pie93, WD95, WD97, MVHV96]. Three-Center [HS91, KJ95, RA91, SPH98]. Three-Dimensional [Art98, DM96, Sta95, Sta96a, Sta96b, Sta98d, Sta98e, DS99, LL99, Sta98b]. Three-Dimensional-Doped [DTM96]. three-electron [Kin99, NM96].

[JM96b, TMH94]. Trends [MM95, SL98]. Triads [SBM97]. Trial [Gui98]. Trianion [Kup98]. Triatom [AS96]. Triatomic [MKDL93, MIW91, NFVM94, RABZ94, Su93, Sut99a]. Triazole [PGS97]. tricyclic [CMA+99]. Tricyclo [Lu99]. Tricyclohexane [Gal96]. Tricyclopentane [Gal96]. triexcited [CVP90, LP98]. trifluoromethyl [KH97]. Trifluoromethylvinyl [KH97]. Triggered [PW97]. Triglycerides [CDMA94]. Trimer [CCB+97, Fou94, GW98b]. trinitroimidazole [CP99b]. Trioxane [BJMT94]. Tripeptide [MK98a]. Triphenylphosphino [Boč96]. Triple [CS98, PG94, WB93]. Triple-Excitation [CS98]. Triple-Zeta [PG94]. Triples [HKC96, NU95, WB94]. Triplet [BS94, CG97a, GS93, HHKM95, Jur97c, LM91, LS93b, STMR97, Gut99b, SC98b]. triplex [PWL98]. Triply [PTP95, RSD97, HOF+97]. TRIPOS [WHF92]. Trisnitroxymetaphenylene [TD96b]. tropolone [WBS99]. Truncated [Sad97]. Tryptamine [NdA93]. Tryptamines [HAEMA92]. TTF [Sta98b]. TTF-2 [Sta98b]. TTF-DCNQI [Sta98b]. TTF-TCNQ [Sta98b]. Tungsten [DFDK99, FDD95, LMC97b, LFD99]. Tunneling [BSS96, BCS96, CR93, DVL+91, EBMS92, Hag92, HZ93, Hag94, Hag98, NBS95, SB97b, SC94, VBD+98]. Twist [RK96a, RK96b, RK96c]. Twisted [MFCA94]. Twisting [MZ93, MGK99]. Two [ASM91, BL77, BBC+94, BMK96, BH71, BGS98, Chr94, Chr97, CE90, DTA+96, De 97, DP97, DQB97, FK94, FS95c, FWT+96, Gal72b, GY95, HBL99, Har98a, HO94, HS92c, HW91, IY99, IP94, KTCN93, LS93a, LMR94, LR94, MW68, MBA97, MRL99, MGLBP95, MD93b, NMM97, NPL90, NYLBNSB97, Pan95, PSO90, PM95, PMN+92, Pie93, PAT93, RML97, RDK97, SB97b, SSD96, SB92, Taş96a, TE96, TZ97b, Thu75, Val96, VBUS99, WG95, WFK97, YO92, ZWZ96b, vvBS96, BSS97a, BMA99, BG98b, BG98c, CB99, DWB98, FR98, GDYY97, HR99, Jon93, KM99b, MHN98, MA99a, NV97a, RDK02, TGS99, Tit96, WDS97, YKN+99]. Two-Body [FS95c, YKN+99]. Two-Center [GY95, HO94, HS92c, IY99, LR94, MBA97, MGLBP95, Pan95, Thu75, Jon93]. Two-Component [HBL99, vvBS96]. Two-Coordinated [ASM91]. Two-Dimensional [BBC+94, FWT+96, Har98a, LS93a, SB97b, SSD96, TE96, VBUS99, WG95, YO92, HR99, NV97a]. Two-Electron [BL77, BH71, BGS98, De 97, KTCN93, NMM97, RDK97, CB99, FR98, KM99b, RDK02]. Two-Particle [ZWZ96b]. Two-Particle-Hole [DP97]. Two-Photon [PSO90]. Two-Point [LMR94]. two-proton [MA99a]. Two-Row [WFK97]. two-shell [BG98b, BG98c]. Two-Site [RML97]. two-state [BMA99]. two-step [Tit96]. Two-Well [Taş96a]. two/one [BSS97a]. two/one-component [BSS97a]. Type [AM98b, Boe96a, Boe96b, BR94, BFH96, BEJ98, BGS98, DTS97,

[GAdAC97, GAdAC97, STMR97]. xylose [FNSV99]. XYSO [GKKM96]. XYZPO [GKKM96].

Y. [Enk97]. Yang [Iva96a, Iva96c, Iva96b, Iva97, Cal93]. YBa [LF95, WL99]. YBasub [SBAD90]. Years [Pul90]. ylacetic [RTKP95]. Ylidene [Cio93]. YN [SG93]. York [Jør92]. Yukawa [HWS92, SF95a]. Yurtsever [Kar96].

Z [Deu98a, Rey90]. Zajonc [Deu98b]. Zeeman [BLG95]. Zeolite [LV98, MBML91, NNMH96, PB95b]. Zeolite/Adsorbate [NNMH96]. Zeolites [KD98, SPG97, SHC+98]. Zero [MD93b, ROL+90]. Zero-Field [ROL+90]. Zero-Voltage [MD93b]. Zeroth [Sie93]. Zervamicin [HMK96a, HMK96b, HMK96c]. Zeta [KZ99, PG94, TKSH93]. Zeta-Function [KZ99]. Zhang [Deu98a]. Ziegler [Sak97]. Ziegler-Natta [Sak97]. Zimm [Jac92]. Zinc [LMMK93, Ryd94]. Zinn [Kum93a]. Zinn-Justin [Kum93a]. zippers [SKM99]. Zn [IK97]. ZnO [MLA93, MALT96, MLT98, SBD+92]. ZnS [MW92, MW92, SZ97b]. ZnSe [MW92, MW92, Por98, Wil90]. Zr [Bec97a, Cun92, CC96]. ZrO [ABCM93]. ZrSiO [ABCM93]. Zwitterionic [PLV92].

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