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Title word cross-reference

(001) [dLdOdAD12]. (100) [MFK+12]. (1 ≤ n ≤ 6) [UDVD10]. (2 ≤ n ≤ 8) [BLRdA+10]. (3 + 2) [WLS+19]. (3 + 3) [LFTL18]. (A = N, B) [ASW13].
(k + l + m = 4) [KYLC19]. (m + n = 3) [UKF+11]. (m = 5, n = 2)
[MHHPR+17]. (m = 6, n = 3) [MHHPR+17]. (n = 1, 2) [Men10]. (n = 1, 2, 3)
[EML+11]. (n = 1 -- 4) [LL11]. (n = 1 -- 7) [CAZ+11]. (n = 2, 3)
[DTEMK11]. (n = 2 -- 10) [WJL+11]. (n = 2 -- 34) [QSLY10]. (N = 28)
[GD11]. (r, s) [Bib13]. (ψ - ψ) [MAW+18]. + [Buc12a, CdAFS+12, DMAB12,
FRNM12, GKT+12, KT12b, LWWZ13, MEEA+13, MPRCEG12, MOH+12,
RSD12, SABA+12, SD12, WZH13, XZL+12, YGL+11, YZ10, ZH12]. 1
[BEM12, DFK16, JW19, PSKV19]. 1/3 [KLQZ15]. 13 [LXD13]. 14 [YD17].
16 [GAPK+19a]. 18 [YD17, GAPK+19b]. 18 [GWZ+14a]. 2
[ABTW14, CPL15, HMA+19, HGB08, I1K14, LLZaH14, LD17, NF11,
PSKV19, SPD+18, SSDS17, YSW11]. 2(N + 1)2 [MC18a]. 2n [BBYZ18].

1
AEKGZ12, BMR+13, DB15, FY11, GNMin12, LCB10, MMA10, Nik11, NRGS11, RVNP12, RNV+12, SD13a, VSS11, Yam10, ZZZ+11. Πu [HHL+12b]. π • π [WLC+17]. πσ* [KGVG11]. pK_a [PBY18]. t [DAU16, SAHAA16]. |Ψ| [GSI10]. q [Agn12]. q = 0 [SM14c]. → [Buc12a, Coo12, GKT+12, LCB10, MPRCEG12, NWQX11, YGL+11, YZ10, ZH12]. rmSU(2) [Bra10]. S [HR12, MMM19]. S = 1/2 [KLIQ15]. σ [LW18, SPIL14, SC18, ZHL+19, CC11b, Ang10, Che12, DCdG10, JLG+12, Yam10]. Σ− [LSL+12]. σ_hole [VBJ15]. σπ [ZXY13, DMWY11]. sp^2 [OCGM+19, PNC19]. \sqrt{3} \times \sqrt{3} [OD16]. T [XCL+18]. \times [PWL+10, ZWWY10]. \rightarrow [GW18, KMM16, ZWL18]. v = 0, 1 [LTFZ13]. v = 0, j = 0 [YZ10]. \varphi [CC11b]. W(l, m; n; \alpha, \beta, \gamma) [LWY13]. ∧ [ZQJW13, LYL11]. X [AGOP18, AM18, BHA19, Kuz19, SB18]. x = 0 [HCL13]. x = 1 [RLW+13]. x = 2 [BCGC12]. X− [Kuz19]. X_2 [BHA19]. Y [Kuz19]. Z [XCL+18].

* [LCB10].


2 [Boe12, EKD12, KK14a, LJK+18, LV12, Men10, MEEA+13, SAHA16, Tan12, WWX+11, Zha14].
2-adamantyl-thiazolidine-4-one [MBBT+12]. 2-amino [RJY+10].
2-amino-3-methylimidazo [MLPT10]. 2-azidoethanamines [SM10b].
2-dichloromethylbenzimidazole [PMC11]. 2-dihydro-3H-pyrazol-3-one [TAY11]. 2-dione [OPP+14]. 2-dioxetanone [dSdS13b].
2-ethoxypyridine [MCC12]. 2-furoic [GIO12]. 2-hydroxy-3-methylbenzylidene [TAY11].
2-hydroxybenzylamine [AFC+10]. 2-methyl-3-hydroxylbutyryl-coA [MFR10].
2-methyl-4-nitroaniline [KC11]. 2-pyridone [HHCA10, MCC12]. 2-RDM [KK14a].
2-substituted [Tug13]. 2.0 [CYC+15]. 200 [KAR12a]. 2D [BCNR18]. 2E [KDC¸12].
2H [FRNM12, VHTEG15]. 2R [CPL15].
3 [CWW+16, LKZ+16, SC12b]. 3-alkylithiophene [BMR+13].
3-aminoacrylaldehyde [NRS+11]. 3-bisphospo-D-glyceric [SLA12].
3-dihydroxybenzylamine [AFC+10]. 3-methyl-3-hydroxybutyryl-coA [MFR10].
3-methyl-4-nitroaniline [KC11]. 3-pyridone [HHCA10, MCC12]. 3-RDM [KK14a].
3-substituted [Tug13]. 3.0 [CYC+15]. 300 [KAR12a]. 3D [BCNR18]. 3H [KDC¸12].
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3-methyl-4-nitroaniline [KC11]. 3-pyridone [HHCA10, MCC12]. 3-RDM [KK14a].
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3-methyl-4-nitroaniline [KC11]. 3-pyridone [HHCA10, MCC12]. 3-RDM [KK14a].
3-substituted [Tug13]. 3.0 [CYC+15]. 300 [KAR12a]. 3D [BCNR18]. 3H [KDC¸12].
4-trifluoromethylphenyl [SAHAA16]. 4-X-2-hydroxybenzaldehydes [EKN10]. 400K [KAR12a]. 4965 [SKHN13].

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9-
[CRSB12].

= [AGOP18, AM18, BLL+13, BHA19, BBYZ18, CWS15, CDL+19, DPDR11, DD17, DHYC19, EMSB15, EMS16, EAV16, GWM11, HNBG15, HNS18, HWL16, JLG+12, KSSK16, KMM16, Kuz19, LJL+11, LC16, LL18, LWL19, LGW11, LXD13, ML+16, MLW10, MZL17, NBL12, PKS+16, PP19a, Pan16, PCD14, PAKA15, RWW+19, RBTL19, SB18, SMC18, SKS10, SPL14, SM17, SYQ+10, TW10, TL15, VO12, WSML16, WZW17, WLL19, XYL+18, XZL+12, XCL+18, YLW+12, ZHL+19, ZCTG18, ZLY+14, dOR10]. =4 [BEM11]. =H [RLTAT19].

activity [BD14, Hat13, MPMCM+11, RCM+19].
acute [PI13].
acyclic [BBKO16].
acylbenzothiazolone [SSTÔ11].
acylhydrazones [Cao17].
acylium [FDMR11].
acylhydrazones [Cao17].
acylphloroglucinols [KM12b, MK10a, MK12].
adamantane [BBKO16, GZ14].
adamantane-based [GZ14].
adamantyl [MBBT+12].
adapted [Ali19b, ANC+15, CB10, SR12, TPCJ+12, VRO+12, WH12, YKN13].
Adaptive [BG11a, BR15, Lya14, MBSMJC18, ZKW17].
addatoms [PP10, WDJ+17].
Added [Fuk12].
Addition [DI11, Buc11b, CAAI12, DP12, DFK16, Dum12, GW13, GMT18, LCM+11, LW13, MJC18, PDNC14, SRL+13, TIN13, TBHL11, WZZL10].
addition-substitution [Buc11b].
additions [SFW12].
additive [KF19].
additives [YZZH15].
Additivity [BMB16, RLER10, Dob14].
address [VVJ15].
adduct [DWGX12].
Adducts [MK10a, BAB+18].
adherence [dOdONM12].
aerogen [EAV16].
aerogen-bonding [EAV16].
affect [VGS10].
affects [GJ18].
affinities [DTMK11, KKT13, KKT14, VF13a].
affinity [CSSK+12, DPK18, DJ18, ESLM19, KKM+12, Kry11b, Kry12b, Shi13, dCSDdMC13].
after [GD11].
Ag [MSOV13, OD16, PAPCMM+16, SZZZ11, SYQ+10, XWC11a, ZPR10, AGG+18, ESBVJY12, JFT13, LRKM10, PK+16, RK14, SRL+13, SQ10, WLL19, ZRR+11].
against [FMP+17, GAI19, KF19, SBKJ18].
AgBr [RS12a, RS12b].
agenda [SG14].
agent [MB14, PPK+13].
ages [Nic14].
aggregates [ATS+11, TFB11, WKE17, ZLE17].
Aggregation [YLH+19, GDM+10, MAD12].
aggregations [BBKO16].
AgOH [KSST12].
agonists [Ser11a, Ser11b].
agostic [HHL12a, HHL14, WLS+19].
AgSi [ZCP11].
ahead [HJK14].
AHHC [dOR10].
aided [GbZA10].
AIM [GWZ+14b, NRHJ11, PK13a, RJY+10, RJA+10, UDVD10, ZZL+11].
Aiming [BBB16]. Al
[CWS15, CDL +19, HHL12a, HHL14, JLL11, LXD13, MILW10, MFK +12, Oni12, Sat11b, TW10, XWC11a, CRB +12, DCDD10, DSZB18, KYLC19, LLZZ10, MCP10, HH11, Pan19, Sat11a, SUL +11, TGD13, WJL +10, PS13b].
alcoholamines [LCT14]. alcohols [MMM +12, SGKG12, SK12a, ZZC12].
AlCoN [AAAM12]. aldehyde [AG10a, LCS +11a, PWH +12, ZSS +13]. Alder
[CM12, Iku17, LW11, MIKH19, ZLWL16, ZXY13]. aldose [SSdS17].
aldehydes [SSdS17]. Algebra [RW12, Lya14]. algebraic
[SCLCPB12, SABA +12]. algebras [WH12]. algorithm
[AFM +10, CGG18, GI11d, IG11, MCP10, SGH10]. algorithms
[CL08, TB15]. AIH [HH11, SLZ +11c]. aligned [HV11]. alignment
[CLL +11]. aliphatic [P113, SN11]. Alkali
[CFC11, Ber13a, HWL16, HWVV18, SHE10, SM14c, UDS19a, UDS19b].
alcoholates [UDS19a]. alkali-based [UDS19b]. alkali [SM17]. alkalides
[DTMK11]. Alkalized [STM18]. alkaloids [JSLH14].
alcanes [GBZH18]. alkenes [ZSS +13, ZFW +13].
Alkenes-3-quinolinocarbonitrides [ZFW +13]. alkenes
[CAAI12, KBJ17, YZZ16, ZYSW17]. alkyl [ESS13, LYW11].
alkylamines [BM13]. alkyl citation [HWW18]. alkyldene
[VGGPdL19]. alkyllithiophene [BMR +13]. alkyllines
[LW15, SLS +15]. alkyl-
[HWW18, LCB10]. all-electron [MPD +10, MPZW10, NDM +12].
aldehydes [MLW10]. all-aldehydes [JHL +18]. alkenes
[XZG +18]. alcohalenes [KB18]. alloxane [KB13].
allenes [KB13]. all-electron [BXR +13, VGD13, XGH +18b].
AlN [AAA12, RJLPDH +13]. AIN [AAAM12]. AIO [SZ11]. along
[IKS08, IKS10, KRG +13]. AIOOH [MMC +19]. alpha
[MTBVR12, SLS +10]. Al
— [TGD +19]. aldehyde [DB13b]. Alternative
[CSTA16, CQCF +14, GZF14, MJ16a, PCK19, SKLC19, Sze18]. aluminum
[Ped16]. aluminosilicate [Ped16]. aluminosilicate [PBM10].
aluminosilicates [DCFD10]. Aluminum [ALK18, AGB19, ALK19, HTM10,
IWE +11, Kar12b, MMC +19, MS14b, MM11, PMH +16, SM19].
aluminum-bismuth-nitrogen [MS14b]. Aluminum-poor [ALK18].
Alzheimer [Bal16, MPTR12]. Am [PMM14]. AM05 [MA10]. AM1 [PI13].
ambient [Ma14, WCDD12]. ambiguity [Fin14b]. ambipolar [MAN5].
America [CJBMMAPR19, MCCGM +19, MNCN19]. American
[HS11b]. amines [KSAK17, LSR +10a, LSR +11, LW15, RZG12, TV13].
Amino [DSOC +13, AM13b, Coo12, CF17, Cza18, DJB10, Jai10, KyH13a,
KSS12, MLPT10, Mit11a, NHG +12, Pog12, QZH13, RJY +10, Ril10, TAY11,
VHTEG15, WHM14, YSW11, ZCC11]. amino-2H-imidazole [VHTEG15].
aminoacetonitrile [CdLdSC18, NC11]. aminoacrylaldehyde [NRS +11].
aminobenzonitrile [NMHPVG12]. aminocarbonothioyl [KDC12].
approximations
[CLXD15, FMMD+10, GZSMFN16, Per18, PBB15, RBD+10, SGL+16].

APSG [JNZ+14]. APSG-based [JNZ+14]. aq [DSZB18]. aqua [BSPK11, MGK19].


arsenide [KP11, UDS19b]. art [NBZG16, PB10]. articaine [PSPS11].

Article [NT15]. artificial [FCC11, YVY+12]. aryl [BMF13, LW15, MHZ18, MSY+12, CM12].

arylamides [DDF+12]. arylation [SH18b, SGL19, Zha15]. arylcarbamates [DDF+12].

ASA [TBST10]. ascorbic [ZYL+13]. Asia [WZ10a]. Asn [ScBSR+10]. AsP [LJSS12].

asparagine [GSZ10]. aspartame [OT14]. aspects [Hop15, IK14, LEU+11, Luz12, PK13b].


Assessing [AM13b, DGA+13, PK13b, TCA10, LYD+18]. Assessment [CC19, LCT14, SBKJ18, Vie17].

BVCAP12, DVP18, JHSG18, KKH18, KSS12, FKDC11, OKR12, PSK+16, PI13, ZST+10, ZT13]. Assignment [LCL+10a].

assignments [LYR+17]. associated [DW12, GI11a, Han19, MBTWR12, WJ11, YKM+15, dCSDdMC13].

association [NWQX11]. assumptions [PIS18]. astrochemical [For17b].


asymmetry [Hop15, JSLH14, LMCZ11, LW13, MMP11, PBB15, SHL+13]. Asymptotic [BEM12, Han19, RBD+10].

Atmospheric [HYZ13, BZZ15, BZX+19, CGIAI12, LLW+12, MXC18, MPGGS19, Var14]. atmospherically [MTS15]. atom [AD17, Bay19, CI11b, DWJZ11, DLG12, DSSM19, Esr18, EM19, FAFR12, G14, GAMM10, GV11, HWW18, HXX15, Ign11, Ign12, JWJ+12, JZZH17, KH10, KKL+16, Kin13, KDA+11, KFIS13, LGIL11, LGNW14, LKLW11,
MFLK11, MAPS18, MNS11, MR18b, Pea11, PSC15, Pup11a, PJ19, RZ17, RZSZ18, RAFFR18a, RAFFR18b, Roy15, Roy16, RRCO11, RR19, SRPD16, SK17a, SKM11, SL13, SS12, TBB+19, TW10, WWHZ13, Zak13, ZS12.

azopyrroles [Jac12]. azosulpha [EAK+10b].


barrierless [DSZB18, dMOB12]. barriers [DI18, SR19, SH18a, SCBP17]. Base [SM13, ACF+11, AZD+11, BTH18, CPF12, CW16, EMSB15, KSS12, Kuv10, LSR+10a, LSR+11, Lad14, MSH13, OM13b, PP14, SMEH15, XSLF12, XTLA13, XTLA14, ZKWZ17, ZBG+19, ZSQ+10, dSTH17]. base-free [ZBG+19]. based [WYM15, XWP+18, YZ13, YZZH15, YKN13, YSW11, ZZZ+18, ZKW17]. bases [BS14, EG10, EAV16, GGP13, JS18, MMR+10, PS10a, XZ11, Yak11, YDW13].

basic [GI11b, GI11c, BM16, KK14a, Nic11]. basicities [VF13a]. basicity [HFL+17, SM16]. Basics [Bae16, Mos14]. basins [HS11c]. Basis [JA12, KY13, KB19, Rud12, VPA11, YFY17, Ali14, ANC+15, ABA11, BL16, BVCAP12, CHH+19, CC19, CML+16, DCZ17, Fuk12, GBK18, GTR11, HH18, Hil13, Hog13, JH15, KRC+16, KPCV18, KUY16, KUT13, Lai11, LV12, LWL+12,
MSNP18, MG12, NDM+12, PCD14, PBR18, RZSZ18, RLFR14, RVO+14, RLZ12, SKTI15, SXH18, SZZ+10, SLZ+11c, SLZ+11a, SLS+11, TCG17, TWR15, UGWL18, UV1b, VSS11, VRO+12, WSV10, YMI14, Zak13, ZF15. bath [YK13]. batteries [Ali19a, AVG19a, KLK13, Kim18, UDS19b].


BEPOX [KZZ13b]. Berry [DMAB12]. Beryllium [NW12, AM18, DZO12b, Nic11]. BeS [DAR+11]. Best [Ish14, CB10]. beta [MBTVR12, PTD+12]. better [BLL+13]. between [ASHF13, AD17, ALMY18, BLR12, BHA19, BL11, BLWJ17, BWB+18, BTH18, BWE16, BB16, CJZJ12, CCL+13, Ccc19, Cha10, CCS13, CDL+19, CF17, DCKCS+12, EKN10, EHKD11, EKD12, EEMSS14, EAV16, Fin16a, Fin17, GXX+14, Gra08, Gra11, GE12a, HCH+18, Han19, HMH+13, HIL19, JEA13, JLS13, Kan11, KdPNN16, KMMS17, Kim16, LKOS17, LdMCD4a+12, LMZ+11, LLG+12, LFTL18, LFP+19, LBdV16, LWC+10, LZD+11, LCS+11a, LCH+11, LCS+11b, LXLL11, MYZ+10, MKF+12, MSY+12, NBL12, NZ13, NAK+17, NBI+10, NL11, NRGSI11, OKK10, PDNC14, PM12, RYM12, RFN+12, RMJ11, RNb+10, RS13, SSF+10, SD16b, SKHN13, Sch15, SM17,
Beyond [Chu12, DCD11, Dob14, EAA17, ZWE12, CTV12, MA10, RB18, SK17a, Var14, VVN+16]. BGl 1 [WHS+13]. BH [Kim13, ZZ+10, SL+11a]. bi [MMR+10, MHHR+17].

bisimide [JR19]. bismuth [MS14b, MHHPR+17, MLK17]. bisphenol [BLWJ17]. bismphenol-F [BLWJ17]. bisphenyls [SN11]. bisphospo [SLA12]. Bistability [SS19a]. bit [Ish14]. bithiazole [SAHAA16]. bithiazoline [Qu13]. BiVO [DWX+16]. Björn [Pyy11, SA11b, Sha11b, SL11]. block [GDM+10, JHL+18, KS19, MAA10]. block-copolymer [GDM+10]. blockade [ZX12]. blocks [LLZ+14, Sza13, XWP+18]. blue [Kry10, LXW+14, SLS+14, SHW+13, TU10, dOR10]. blue-emitting [SHW+13]. blue-green [SLS+14]. blue-shifted [Kry10]. blue-shifting [dOR10]. BN [LGHL11, BSS15, FKL+12, GLT13]. BnHn2 [LCZ15]. BnHn2- [LCZ15]. bodipy [TPT19]. body [ARG11, BSO16, DLP17, Fri12, GR11, Hog13, IM15, KRG+13, LV12, Lin14, Lya14, Per10a, RAN18, RAGM10, SK17b, SIB+13, SHKS15, Zak16]. body-fixed [IM15]. Bond [CP13, FC19, GRLA18, HS15, Mar11, MPCMCM+11, RL12, SB10b, ZZC12, ZFC12, dFR15a, AV19, AGB19, ABKJ18, AD17, AG19, ASK15, AMMB+18, BCP10, Bia15, Bou12b, BWB+18, CC11a, Che12, CYC+15, Coo12, CF17, DL17, EKN10, EMS16, FGD+19, FKC12, GIO12, GI11b, Gin10, GWME18, GPM+15, GZBH18, HNH+12, HHL12a, HHL14, HAX+18, JLG+12, JE10, Kal18, KZA+17, Kan18, KK14a, KK11a, KM12c, KN15, Kuz19, LZZ+11, LW18, LW15, MNV+17, MTR+19, MGB18, MBSMC18, MBA+19, MML11b, ND11, Nail2, NHB12, NRGSI1, NRIP+11, NRHJ11, OKR12, OK16, OHDA13, PCMG12, PCK19, RJA+10, RI19, RB11b, RKCK19, SS10, SSK+12, SH18b, Sch10b, Sch13, SMEH16, SRA+11, SCL19, SBD18, SC18, TL15, Tob19, TCA10, VVJ15, WCGD12, WTW+15, WLC+17, XHZXXZ10, XX12, XCD18, YYY+13]. bond [YL10, YS18, YZZ16, ZAE10, ZZX10, ZCC11, ZYL+14, dFR15b, dSNB08, LCM+11]. Bond-dissociation [SB10b]. Bond-extended [MPCMCM+11]. bonded [CdLdSC18, CCP18, DLM12, DMBL16, DB15, GCD13, IKS08, IKS10, KS18, LJJ+11, LWW+11, MT10, Mit11a, MS14c, OA13, RNE10, SGK12, SPI14, ZLZ+14, ZFS+11, dSCC12]. Bonding [Con10, Mil12, TFM19, XWC11a, ZPR10, ABM+19, AMK10, AG19, BHA19, BMM+19, BG11b, Bucl10, CLXZ12, CPF12, CG12, CCL+16, Cha10, CNSK11, DMS+10, DB15, EPS+16, EAV16, Fin14b, FC19, GI14, GLXL18, Gin10, GORW19, GPM+15, HSYM11, HYD11, JN13, KK13, KdPNN16, Kry10, KM19, LRY+17, LFP+19, LWL19, LW18, LBdV16, LYD+18, MCCGM+19, MS14a, MPD+15, MT10, MC12, MKM11, NZLG15, NE11, Pan16, PK13b, RJY+10, Riv11, RCS10, SM19, SJZ+18, SYY16, SC18, UDVD10, WSLM16, WJ11, XZYS10, YZW15b, YRJ+11, ZFC+17, dOdCMuDLR11, CFV18, GAPK+19a]. Bonding/ [CFV18]. bonding/antibonding [CCL+16]. bondons [PO15]. bonds [ABS13, AKHS13, AM18, ALHC18, BLR12, BL11, CG12, CDL+19, DR18, DLM12, DLLA10, ED16, EEMSS14, HB14, IROW10, JLZ+17, KKC14, KKG12, LLF+12, LG+12, LZD+11, LLZ+12, MK11, MK12, MAT19, MJ16b, MGB18, MB15, NBL12, NZ13, OS10b, PRFR17, RRVJ10, Ril10, SSI+10, SSK+12, Sch13, SMP10, SIS+08, SPI14, SS11, SM14a, SW12, SCZH16,
TKS11, XCL+18, YSS+10, YYI+13, YGLL10, YWH+12c, ZYL+19, ZLWZ16, ZYL+14, ZS13, dAVdM17, dLRR11, dOR10. **Book** [Ban12, Brä12, Kry11a, Li11, Lin12, Mas11, Mor13, Mue12, SGJ10, Sch10a, Tay12]. **boosters** [HEVMSA+19]. **borane** [LCZ15, MFOH18, MC12]. **boranes** [GWM11]. **borazine** [Kal18, RLTAT19, STM18, ZYL+19]. **border** [AGOP18, CN12, GMT16]. **borides** [CFC11]. **Born** [BPL13, GVPCK10, RSM12, RAN18, SK17a, Sur12, VVN+16]. **borofullerenes** [YLH+19]. **boron** [ALHC18, BCGC12, Buc10, DWGX12, ES17, Esr18, FZX18, GAMM10, HIL19, HNBG15, KC19a, LC13, LCI2, Mar11, MJSC18, OTV+16, PPDF11, RRCO11, TNT18, TCS12, UDS19b, WG18, XYL+18, ZDF13, ZCG+16, YGLL10]. **boron-rich** [HNBG15]. **boron-arsenide** [UDS19b]. **boron-nitrogen** [KC19a]. **boron-rich** [TCSD12, WG18]. **boron-arsenide** [UDS19b]. **boron-nitrogen** [KC19a]. **boron-rich** [TCSD12, WG18]. **boroxine** [Kal18]. **boroxol** [LFP+19]. **Bose** [DCD11]. **Bound** [Agb12, AY15, PGMGRM15, TD19, DSSM19, Fin16b, FDA16, FRGC10, GWHH17, KH10, LDADB+15, ONK+13, Ril10, WC14]. **Bound-states** [Agb12]. **boundaries** [WLH+19]. **Boundary** [LZ12, CW13b, MFLK11, UYN+13]. **bounded** [LLP17]. **Bounds** [MC11b, PR10a]. **Box** [GZSMFN16, NCNC+18, GZF14, Lnu13a, Lnu13b, Roy15, Tou13]. **boxed** [RAFR18a, RAFR18b]. **bpy** [DS11]. **Br** [DVDBM11, EMSB15, EMS16, JLG+12, Kuz19, LCL+10a, LMZ+11, LLG+12, RLTAT19, SB18, SZL+14, TL15, WZW17, XYL+12, JLZ+17, LWL19, OK616, TSL11]. **bracteatin** [KK11d]. **Bragg** [Zag11]. **branched** [SPD+18]. **branching** [MOY13, RSL10, TSL11]. **Brändas** [Ban12]. **Bravyi** [TSS+15]. **Brazilian** [DC10, DC12]. **Br** — [LLG+12]. **BrBr** [LG11]. **BrCl** [JLZ+17]. **BrCN** [BM10]. **breaking** [AGB19, DLCB15, SSK+12, SC18, Tob19, WL18, YIY+13]. **Bredt** [Iku17]. **BrF** [JLZ+17, Wu11]. **BrF-HX** [Wu11]. **BrHBr** [GR18]. **bridge** [CLMY12, HSS18, KyH13a, Na12, Na13, SSK11]. **bridge-acceptor** [SSK11]. **bridged** [MNP19, ZLR+12, ZLS+18]. **bridges** [ATS+11]. **bridging** [MG10]. **Brief** [Ano11a, BC15, BC16, Mai14, YZ13]. **Brillouin** [BG11a]. **broad** [FCS13a, FCS13b, TZ11]. **Broder** [PR11a]. **Broken** [FDNR10, SC10a, CR18, GFRdG11, Tob19]. **broken-symmetry** [CR18, GFRdG11]. **brominated** [MFB11]. **bromine** [FGD+19]. **bromo** [OA13]. **Brønsted** [GI14, RDB19]. **brookite** [GP13a]. **BS** [YGLL10]. **BSE** [RAMB18]. **B** — [MGB18]. **bt** [Qu13]. **Bu** [GWM11]. **buckyballs** [GKGM18]. **buckybowl** [LZW+15]. **Buckycatcher** [DI15]. **build** [GBK18]. **building** [JHL+18, KS19, LLZ+14, MDC15, MSOV13, Sza13, XWP+18, CNBPR+11]. **bulk** [TFB11]. **bundle** [GWME18, JE10]. **bupivacaine** [MP12]. **butadiene** [SKTI15]. **butadiynol** [SBAT16]. **butadiynyl** [KI12]. **butanetriol** [LL17]. **butatrienone** [SBAT16]. **butene** [IK14, TFA10, ZPB12]. **butyl** [AMAC12, MFK+12, WZZL10, dOLdI13]. **bzq** [ZQIW13].
C [AM18, Ban12, BDF+18, BCP10, BGFD14, BBYZ18, yBZfC18, CJMC19, DQZF12, GWM11, GZW16, GB13, GCD13, JLL+18, JLG+12, Kal18, KN12, KN15, LKN13, LCS+11a, MLY+16, MGD11, NBL12, OGvSG18, PAKA15, PP14, SUL+11, USL+13, VF13a, VLK+11, WLZ+12a, WLZ+12b, WZ17, WSL+11, YK11, YZL+10, YLZ+17, YL11, ZQJW13, ZHL+19, ZW15, ZLWZ16, ZCTG18, TSKN12, YB11, BHA19, yBZfC18, CCEGK12, CWL+13, CRSB12, CTDOLA10, DFK16, DSFT17, EML+11, FBRBR12, FBO+11, GB13, HV11, HLB19, HHL+12b, IMS+13, JB18, JCCZ12, KWC10, KZA+17, Kan11, KK11b, KK12a, KI12, LCL+10a, LBY+14, LZW+15, LCZ15, LX13, LDAA+11, MNV+17, MSS11, MIN13, MS17, MPGG19, MC18a, NL11, NMIP14, Nk11, OCL+18, PTS+11, PAKA15, RR11, RRCO11, SBA16, Sat11b, Srl19, SCTW10, SW12, SZY17, SC18, TZD+19, TG13, TSKK17, WCS+13]. C [WZW17, WWGW18, XCY15, XCD18, XZG+18, YS18, ZPM10, ZLWL16, ZJC+13, DZO12b]. C-H [YS18]. C1s [LDBF+12]. C2h [KS18]. C60 [DI10, GHGF12]. C=S [JLG+12, JLG+12]. Ca [VO12, WCY+10, XZZ+10, YLW+13, CRB+12, CLMY12, DTEMK11, GR11, MPD+10, MPTZ13, SBB16, VPFD10, YYI+13]. Caballol [dGR14]. CACA [Ser11a]. cacao [dAGNJT12]. CaCuO [Fuk12]. caffeine [LCG12, PRG+10, ST15, PRG+10]. cage [yBZfC18, CS13, DI18, GAPK+19b, JL12a, SL10, WLZ+12a, KK12a]. cage-like [JL12a]. caged [PAKA15]. cages [NW12, XYL+18]. calcite [SC11]. calcium [Ish14, RCGLV+14]. calcium-doped [RCGLV+14]. calculate [ZLE17]. Calculated [SPO+11, Dw13, FKL+12, MKF+12, VMC11, WWC17]. Calculating [FHYc11, KC11, WB17, ARH+13, CML+16, MGK+11, SA11a]. Calculation [FZC14, KKS+11, MHO+15, Rit12a, SHS+13, VLFG12, VO11, YSO12, AM12, BVCAP12, BBYZ18, Boe12, CP10, DK13, FLCHL10, FBM+10, FSB16, GWZ+14a, GCDNGS12, HMI+15, Han19, IK18, KMK+16, KHH10, Kri13, LBLqD+19, LK15, LSKM19, MGK+12, Mam13, MA12, Mit11c, dMOB12, PS10a, Per10b, PCR+11, Rit12b, SBM16, SMGZF19, ST15, SRASZ16, TTT13, VFI13a, WZH13, XCD18, YK13, YMI14, YH14b, YLYC18].
calculational [SC12a]. Calculations [KH10, KV11, LKJ13, SR19, TWHZ14, dHLd12, AV19, AK17, AFA13, ADB10, ACMRN10, AGG+18, BCK19, Bas11, BB10, Bou12b, BJ12, Buc11b, Bud12, COCF+14, CK17, CSTA16, CFC11, Dau16, DGL515, DAE+12, DWX+16, DZO12e, DZO12a, DFF+13, ESS13, Eng16, FSK+11, GAPK+19b, GVPC10, GsAY11, GZF13, Ghi13, GJ18, GE12b, HK11, HHCA10, HH18, HS11b, HL19, HNBS18, HZS14, IKC18, JHS13, KAR12a, KK14a, KG17, KKR+17, KPCV18, KSS12, Kim13, KJ15, KJ16a, KJ16b, Kin13, KYH+13b, KPH+12, KKG12, LRP+11, Leh19a, Leh19b, Leh19c, LCL+10a, LC16, LLYW+19, LCK+16, LLZ+12, LNI12, MCCGM+19, MJ16a, MVC13, Mit11b, Mit11a, MFLP12, MSY+12, MPT11, MPTZ13, MJM19, NS19, NKWT19, NMSR14, NZLG15, yOF15, OKK10, OCGM+19, OPP+14, OH19, OSJ+12, Pan19, PP19a, PK16, PBR18, PB10, RS12a]. calculations
CASPT2 [BDFM10, BDR12, ČFČ11, GLOGM+11, KZZ13a, LCL+11, LGP+12, MR11, Pul11, RS12b, SKTI15, SZZ+12].

CASPT2/CASSCF [BDFM10, DAR+11, GLOGM+11, Lar11, Ols1a, PE11, RS12b, RSNI12, SZZ+12, SBL11].

CASSCF/CASPT2 [SZZ+12, BDFM10].

CASSCF/MRCI [DAR+11].

Catacondensed [RB08, RB11a].

catalysed [SMRK18, ZYSW17].

catalysis [BvWG14, KJ14, MMM+12, MCRS16, Pis18, Sic16, SLS+15, XDM+10].

catalyst [ENV15, Esr18, EMI9, GB18, Hog13, JXX+15, LCM+11, TM19, Var14, ZQW+17, ZBG+19].

catalyst-free [ZBG+19].

catalysts [BAB+18, TFZ+15, WR14a].

Catalytic [BD14, PM17, SS18b, AGOP18, BGFD14, CLY12, DMBJ15, ED16, GGZZ16, GSB10, HSN+11, HSYM11, LPOP12, MLW+14, MMP18b, NEEV15, TK16a, TTD13].

catalyzed [XGH18a].

catalysis [AKC10, AZD+11, CAPGAIG18, CWZ+10, Che12, GCZ+14, HZZ+19, JL12b, JSLH14, KUTS10, LGM+18, LW13, LQ13, YLR+17, LLF17, LD17, LTL18, LFTL18, LMCZ11, LCZL11, LW13, LW15, LKZ+16, MPGGS19, MCC13b, PRFR17, SH18b, SHL+13, SR11a, SLS+15, TTD13, TFA10, WML10, WWLZ17, WZZL10, WRW+18, XZG+18, YS18, ZCZ+12, ZSHL14, ZQW+17, ZSS+13, ZLY+14, ZPW16].

catechin [MKHM11].

catecholamines [MBTVR12].

cathode [KLK13, Kim18].

Cation [ZLWZ16, ATS+11, Ber13a, BMX+19, DWJZ11, DAE+12, HV11, LCL+10a, LLC+11, MMMM12, MS14c, ONBP11, Oni10, OCGM+19, PDR+14, PsS10, SPSA11, SZZ+12, XZL+12, YM12, ZFC12].

cationic [BCGC12, FTB11, ZQJW13].

cation-exchanged [PvS10].

cation-exchange [PvS10].

cation-exchanged [PvS10].

cation-exchanged [PvS10].

caused [HYH+10].

causes [ABP13, MFM18].

causing [MFR10].

cavernous [CJMC19].

cavities [MGK19, Pup11a].

Cavity [PCR+11, OPC17, RAFF18b, RAFF18a].

CBS [CFOC+10, VF13a].

CBS-Q [VF13a].

CBS-QB3 [CFOC+10].

cc-pV5Z [SLS+11].

CCH [EMS16, LZZ+11].

CCI [SKS11, LGW11].

CCSD [CK13, VV13, BL12, CPF+11, DVP18, DdOS16, SLS+11, TD19, VV12].

CD [SZY17, ASHF13, XZZ+10, XWC11a, LKLW11, XWC11a].

CDO [ADR+18, SAHG11].

CdS [XWC11b].

Ce [WLG+11, WSL+11].

cefotaxime [LBM11].

Cell [KMT+12, CWB+13, JK12, LGS+16, MANP17, QJ13, SSS15, TGRP19, WLL+13, WWB+14].

Cell-penetrating [KMT+12].

cells [AGJ12, BDG17, FFDP16, FM16, cLqFtW+14, LYS+19, MY17, PMAP12, SG19, TZ11, ZSAP11, Zha17].

cellular [Kuv10].

cellulose [FNBK17].

center [Buc10, Buc11a, CRSB12, CN12, Hog10, HS14, Koc13a, MSNP18, Tal11, Yam10, YD17].

centered [GAPK+19a, KFS13, Zak13].

centers [ASD14, YGLL10].

centrifugal [CLXD15, IIH16, ZLJ11].

centrosymmetric [KPT+17].

century [Pup11b].

CeO [QCB+10].

ceria [KJ14].

ceric [BSPK11].

cerrado [CCA+12].

cesium [MMR+10].

CF [IAyL14, Mor11, Mor11].

CFCI [dOdCMuALR11].

CFP [KyH13a].

CGR
[HXDY16]. **CH** [ACMRN10, CdAFS⁺12, CRSB12, DQZF12, LJJ⁺11, LXLL11, Men10, NBL12, dMOB12, TSL11, XWCY11, BMR⁺13, BHV⁺11, BZZ15, BXZ⁺19, DS12, DZ11a, FRNM12, GZMC11, HHL⁺12b, KAR12a, Les12, LP10b, LKLW11, MEA⁺13, dMOB12, Puz10, SK14, SD12, SZZ⁺12, STL12, SLZH12, TSL11, VLK⁺11, WZH13]. **CH/** [BM10⁺13]. **chain** [Cal10, DSCO⁺13, DW12, EPS⁺16, IKS08, IKS10, Lak10, LGL⁺19, PP19b, WW11]. **chains** [BEM11, CEM14, CEV10, CFGC11, DSFT17, MAT19, NRI15, PL18a, TIKL13, WZ10b, Yak10, ZZ12]. **chalcogen** [BHA19, EMSB15, EMS16, MZLM17, Sch13, ZFS⁺11]. **Chalcogen-bonded** [BEM11, CEM14, CEV10, CFGC11, DSFT17, MAT19, NRI15, PL18a, TIKL13, WZ10b, Yak10, ZZ12]. **challenged** [Li15]. **Challenges** [DE18, KO14, KJ14, FAK19, NBZG16, Pie11]. **chameleonic** [SSK⁺12]. **change** [DSWL11, KCK14, MS12⁺18]. **changes** [FBD⁺13, GMP⁺11, YSG10]. **changing** [DLG12]. **channel** [AGRI⁺12, LZF13]. **channel-charybdotoxin** [AGRI⁺12]. **channels** [Les12, RBGG18, STL12]. **chaos** [KC18⁺]. **chaos-driven** [KC18⁺]. **chaotic** [Gan14, YW16]. **character** [CCL⁺16, CFV18, CJMC19, CAO18, MHOG18]. **characteristic** [KK12a, MKHM11, OCL⁺18]. **characteristics** [EAA17]. **characterizing** [MAW⁺18]. **characters** [CC11a, MMF⁺13, XWC11a, YMY⁺13]. **Charge** [CS17, DPRK12, EPS⁺16, GI11a, GWME18, GHS12, JdL08, KT12b, MHOG18, SSK12, SJ14, Zen11, AS19, BHV⁺11, CLMY12, DTFK15, DS11, ELC08, FSBA12, Gao12, GNM⁺12, Gin10, GGD12, GHCMQ17, JR19, KUS19, KBMM10, LYS⁺19, LXW⁺12, MGK⁺12, MSG16, MANP17, MPL⁺11, NDH10, NTV⁺14, OK19, PK13a, PSC15, PETB18, QJ13, RS12a, SSK11, Sch15, SRA⁺11, TCG13, TCS10, WDJ⁺17, WDS19, ZY13, ZB18, dCDC⁺11]. **charge-bond** [Gin10]. **charge-dependent** [PSC15]. **charge-dipolar** [ELC08]. **charge-solvated** [CLMY12]. **Charge-transfer** [Zen11, FSBA12, TCG13, ZB18]. **Charge-transfer-to-solvent** [CS17]. **charge-transport** [ZB18]. **Charged** [TGRP19, BGM15, BM13, CAZ⁺11, DCBB11, EPS⁺16, HITU16, KWWH18, LZ12, MMBK12, RTG⁺19, SS10]. **Charged-cell** [TGRP19]. **charges** [CG12, CB10, GSR12, GFRdG11, KKS⁺11, Sch15, TMC18, TC12, ZZZ⁺18]. **CHARMM** [HSS⁺11, PSS11]. **CHARMM-based** [PSS11]. **charybdotoxin** [AGRI⁺12]. **CHBr** [WZH13]. **CHCHCF** [lAyL14]. **CH** ... [EAA17]. **Checking** [HMH10a]. **chelate** [MH18]. **chelate-aryl** [MH18]. **chelated** [ZPW16]. **chelates** [NZAV10]. **chelating** [FND⁺10, NFO⁺11]. **chelation** [Bal16]. **chelator** [DP16]. **chelators** [MP12]. **chelotropic** [CJGT12]. **Chem** [BR16, COP16, HS15, Man16, dFR15a]. **Chemical** [AGNS14, Br14, DVC14, Joh17, KKH⁺13, LLM13, MNE⁺13, NYA⁺13, NDLC19, PM16, SCI0b, TIN13, TM13, TCCI10, Tsu15, Zh14, ABS13,
ASMP15, AD17, AMMB+18, BF11, Ba16, BL10, BL11, BG11b, Brä13, BVRM10, CJBMMAPP19, CKL16, CLXD15, CFGC11, CPAT11, DKZ+10, DPK18, DSL15, DPRK12, DFK16, DMS+10, DLM+11, DMBL16, DSBFT17, EAK+10b, EML+11, EMED+12, EMEDP15, FBO+11, FBD+13, Gal11, GP13a, GRCGRRHT19, GFPAV19, GA19, GI11a, GhZA10, Gru17, HMA+19, Hop15, HAX+18, JN13, KWC10, Kal18, KBGC12, KMK+16, KM12c, KUTS10, KK11d, LZZ12, LRY+17, LL17, MC11a, MPE15, MTR+19, MC14, MG12, MQA17, MKM11, MBBT+12, MML11b, MGP16, NC11, Na12, NZ13, Nêm14, NVPCJ+13, NRP+11, NJA+12, OS10b, OWD18, OSJ+12, ÔEB11, PWY+18, PO15, Qu13, RLW+13, RGTS11, RNE10. **chemical**

[RMP+14, RR19, RBTL19, SSI+10, SSK+12, SAG13, SBEH11, SKHN13, SC12a, SW10, SN15, SM19, SC10a, She14, Shi13, SIS+08, SKM11, SR13, Sko16, SFY12, SBKJ18, SRA+11, SK10, SSB+12b, TFBG14, TYN13, Tap15, TMC18, TSFK17, UTTN13, UJSJ13, VOK+18, V011, VO12, WYM15, WLD+10, WLLW14, YNL18, YSS+10, YYY+13, YB11, ZBK15, ZZC12, dHLDs12, vL13, vLRRK15]. **chemiexcitation** [dSM19a].


chemosensor [LWZ+14]. CHF [STL12]. Chiral [YWR+18, BâGTG11, CPL15, KGYG11, LPM+11, LMCZ11, LW13, QCW+12, SFW12, WTZ+11, YYW+12, ZSS+13]. chirality [Luz11b, SD13a].

chromophores [HSS18, LDKB15, LXW+12, PJP08, ZWLC12]. CI
[ADB10, MdAdCS12]. cinchona [JSLH14, LMCZ11]. cinnamates [PSK+13].
cinnamic [AEKGZ12, PSK+13]. cinnamoyl [AEKGZ12]. circular
[DLRFY10, PCR+11, SB10a]. circumscribed [ACT19]. cis
[BSM+15, Bud12, FMKJ14, GLOGM+11, HWWW18, KZZ13b, TMC18,
CC11a, LCB10, LZ10]. cis- [FMKJ14, KZZ13b, TMC18]. cis}{-1 [CC11a].
cis}{-11 [LCB10]. cis}{-13 [LCB10]. cis}{-7 [LCB10]. cis}{-9 [LCB10].
cis-trans [BSM+15]. CK2 [DPK18]. CI [DS12, EMSB15, EMS16, FBO+11,
GB13, HJRO13, HNBG15, JLG+12, Kuz19, LMZ+11, LLG+12, LWL+12,
LCS+11a, MZLM17, MEEA+13, MPRCEG12, RLTAT19, SB18, SKS10,
SD12, SPI14, SYQ+10, SZL+14, TL15, WZW17, XZL+12, DZO11, KZA+17,
LLBL13, LdAA+11, Ma14, MGB18, SM14b, SC18, ZYS10, YGL+11].
Claisen [EM17, YY18b]. clam [CHL+19]. Clar [RB18]. Clarification
[CHSO13]. class [GMGRMP12, HS11c, KM12b, Mar12]. Classes
[TÅ10, VOK+18]. Classical
[BM16, KC16, BTH18, Cho16, Cho19, CP11, DW12, Dw13, Liu15a, Mak15,
MLB+10, SPSA11, XLLZ10, YZ10, Zak16, Men15]. classical-map [DW12].
Classification [AA11]. classifications [LQZZ12]. clathrate [LB19]. Claus
[SR18]. ClC1 [LGW11, MZLM17]. cleavage
[KRH13, LW15, QZH13, SRA+11]. CIF [SPI14, SCZH16]. climbing
[SSB12a]. close [FSQ+11, HNH+12]. close-carborane [FSQ+11]. closed
[JE13, KK13, MSR11, STM18, dSDs13b]. closed- [JE13]. closed-shell
[MSR11, STM18, dSDs13b]. closo [LYR+17, SALK19].
closo-dodecaborate [LYR+17]. closure [YY18b]. cloud [FT15]. clouds
[BN12]. clue [PSK19]. Cluster [TC10, AHC+18, Ali19b, BN12, BDFM10,
BP13, BVPI3, BVPI4, B BB+12b, BA13, BAB+18, BJ12, Cam10, Cam12,
Car19, DZO12c, DMIL16, EFO11, EO11, Fer11, GLF+12, GWZ16, GP13b,
GD11, HCH+18, HFB19, KP11, LP10b, LSR+13, Luz08, MMBK12, MPT11,
MC18b, NW12, PWL+10, PCV19, PB10, RSN12, REFGPP+16, RWV+19,
RMY+13, SR12, SYK+12, SKS+12, SZS+10, SS18b, Sto18, Sza13, THL+15,
TCS12, Tob19, TGA+11, Var11, VVAO12, VVVB10, WWCG17, WWQG17,
YY18a, YYI+13, YIY+13, YKN13, YT14, ZE18, ZW15, ZCTG18].
cluster-configuration [Ali19b]. cluster-continuum [REFGPP+16].
clusters [AGCV15, ATL+14, AGB19, ALHC18, BD14, BGC12, BPT12,
BGMD15, BvWG14, BGL+16, BPSM12, BJdLMAV12, CSDK12, CAZ+11,
CF11, CCP18, CTW12, CD12, DVDB11, DPK18, DTEMK11, DYHC19,
DQZF12, ESQ16, EBH11, FTB11, FMC11, GR11, GP13a, GAPK+19b,
GGD12, GKG18, GD11, GFRG11, GWJ12, HDQ+13, HLS+14, HJ13,
HFB19, IWI+11, JFT13, JL18, Jen13, JL12a, KP11, Kar12b, KSS16,
KYLC19, KSG+12, KRG+13, LKN13, LL11, LFP+19, LC15, LMC19, LG15,
LSCM19, LHL+15, MJ16a, MBKH19, MLW10, MCP10, MJ14, MMV+19,
MJS18, MD11, MPBR+10, MRR13, MMRA10, MW15, MCK17, NG11,
Nes11, OKK10, PMH+16, Pop19, PAPCMM+16, QSLY10, RIV11, RF10,
RCGL14, RGR12, SFA19, SJZ+18, SIB+13, SR13, SBB16, SCS15, TZD+19,
TW10, TFMC19, TPCJ+12, UKF+11, VSMK13, WJL+11, WCS+13.
clusters [WJL+10, XGH18a, XWC11a, XWC11b, XF19, YSK+12, YGLL10, YZZ15b, YJ17, YZ12, YC13, ZWSF16, ZRR+11, ZCW16, ZCP11].
clusters-continuum [DQZF12].
CN [EMSB15, LZZ+11, Oni12, ZLWZ16, CP10].
CNaY [LZZ+11].
CNC [Zha10].
CNH [Tap15].
CO [BGFD14, BAA+18, BDR12, DPDR11, DWPK14, GGJD13, WZC+12, WRW+18, Kim19, VDGI3, YL11, BD14, BGFD14, BldV19, CRSD12, CCS13, Esr18, EM19, FTB11, GSB10, HDC+11, LCT14, LZW+18, MPM15, MPP+18b, RDB18, RDB19, RBT19, SCLCPB12, SAHA12, SLSZ13, Srl18, Srl19, SCTW10, WLG+11, ZWC+12, ZCW16, AAA12, CRB+12, GZMC11, Kim18, MRT11, NKWT19, ZYSW17, WRW+18].
Co [GZMC11].
Co-based [Kim18].
CO-photolysis [BGFD14].
CO/WRW+18. Co/Ni [AAA12].
CoA [LZZ12, MLW+14, MFR10].
coadsorptions [SR19].
cobaloxime [JL12b].
cobaloxime-catalyzed [JL12b]. cobalt [JL12b, SS19a].
COCH [Men10].
cocrystal [DGR+16, LZZ+13].
cocrystallization [KAOB11].
coding [FMPM+14, GCK+17, MM L+16, dMOB12].
coding [YHL+13].
coefficients [AFM+10, FLCH10, FB10+10, KH12].
coenzyme [SLS+10].
cofactor [LZZ+12].
cofactor-independent [LZZ+12].
cofactors [KGK13].
cognition [Val13].
collaboration [FMPM+14, GCK+17, MM L+16, dMOB12].
Collins [Sit15].
Collective [MLDP10, BM10].
collinear [SABA+12].
Common [VSL+15, ESLM19, LCH14].
compact [LQZZ12, LLZaH14].
CoMFA [MGK+12].
Comment [BR16, CK13, COP16, FKBG19, Fer19, HS15, KBG17, LAd14, Lm13a, Man16, MBSAG16b, PS14, Tou13, VUC13, dSSF16a, dFR15a, HYJS19, PS13b, VV13, VV12, VV13].
Combination [KYH+13b, SN15, Buc10, CK13, DQZF12, SZS+10, SLZ+11c, SLS+11, VV12, VV13].
combinations [Boe12].
combined [IK18, SJC12, TAY11, KP11, MLDP10, N13, Tan13, ZLYW13, BBB+12b].
combines [WZX15b].
Comparative [BLRdA+10, BO11, CLH14, DTEMK11, FDG18, LJJ+11, LL19, LL17, MMF+13, NS10a, PI13, SD16a, dAGNJT12, CCBR+12, FFF10, HNN+12, KM12a, KKM+12, LCC10, LLZ10, ONBP11, PRPU+13, RS11b, YM13, ZLZ+14, ZLY+14, dSDPG11].
comparing [HXDY16].
Comparison [AM13a, BPT12, CDSK12, Han19, JdOS16, MR11, RALK18, SSP+17b, SMN13, UV18b, YFL6, ZHL+19, ABLT11, BLL+13, BGKK16, CCCI9, GP13a, HDQ+13, Kd11, Kc16, LdBF+12, LZFZ13, OKR12, dSPMSF18, SD13a, Sch13, SG19, SBKJ18,
VOK$^{18}$, FMCA$^{11}$, FC$^{19}$, RCM$^{119}$, SCZH$^{16}$, ZZL$^{11}$. Comparisons [CA$^{17}$, PGG$^{12}$]. compass [ZBK$^{15}$]. compatibility [Fin$^{17}$]. compensating [FUE$^{12}$]. compensatory [Chu$^{12}$]. Competition [GE$^{12a}$, SM$^{17}$, TL$^{15}$, GHS$^{12}$, LFP$^{19}$, NRGS$^{11}$, YZZ$^{16}$]. Competitive [LLG$^{12}$, AMMB$^{18}$, SBK$^{118}$]. compilation [TB$^{15}$]. complementary [Yak$^{11}$]. complemented [WJY$^{15}$]. complete [CHH$^{19}$, CC$^{19}$, GS$^{10}$, LV$^{12}$, SGB$^{11}$, SXH$^{18}$]. Complex [GLT$^{13}$, IA$^{13}$, JH$^{13}$, KBF$^{13}$, ONK$^{13}$, BSS$^{16}$, Bou$^{12b}$, Cho$^{16}$, DSD$^{18}$, DI$^{15}$, DZO$^{12b}$, FDN$^{10}$, GRL$^{18}$, GR$^{10}$, IKC$^{18}$, JLG$^{12}$, JR$^{19}$, KRG$^{13}$, LZ$^{12}$, LV$^{16}$, LLG$^{12}$, LSR$^{13}$, Lbd$^{16}$, LDADB$^{15}$, LKZ$^{16}$, MNC$^{12}$, MIN$^{13}$, MMT$^{13}$, MSBF$^{18}$, NS$^{10a}$, NTGC$^{19}$, NBI$^{10}$, NMIP$^{14}$, OAA$^{19}$, PEA$^{12}$, PWY$^{18}$, Puz$^{17}$, Qu$^{13}$, RW$^{11}$, SS$^{19a}$, SY$^{10}$, Sat$^{11b}$, Sic$^{16}$, SLS$^{15}$, VDG$^{13}$, VPOG$^{19}$, WRW$^{18}$, XZ$^{11}$, XCD$^{18}$, XCL$^{18}$, YSS$^{10}$, YI$^{10}$, YSY$^{12}$, YS$^{13}$, YW$^{16}$, ZSASS$^{13}$, ZSHL$^{16}$, dCSDdMC$^{13}$, dOdCMUdALR$^{11}$. Complex-scaling [JH$^{13}$]. complex-valued [YW$^{16}$]. complexant [XWC$^{11}$]. Complexation [ESLM$^{19}$, SHE$^{10}$, ZKK$^{11}$, ZAE$^{10}$]. Complexes [ALMY$^{18}$, GHGF$^{12}$, AC$^{19}$, ADR$^{18}$, AM$^{18}$, BHMN$^{19}$, BPG$^{10}$, BAP$^{12}$, BHA$^{19}$, BZB$^{13}$, BLd$^{19}$, BPK$^{19}$, BCS$^{12}$, BB$^{16}$, BS$^{12}$, CRB$^{12}$, CFP$^{12}$, CTW$^{12}$, Con$^{10}$, CLMY$^{12}$, CADG$^{18}$, DSD$^{18}$, Den$^{19}$, DPD$^{11}$, DG$^{19}$, DC$^{10}$, DD$^{15}$, ED$^{16}$, ESS$^{13}$, EMSB$^{15}$, EMS$^{16}$, FBR$^{12}$, For$^{12}$, FBD$^{13}$, HS$^{11b}$, HL$^{19}$, HYD$^{11}$, HZZW$^{11}$, JW$^{19}$, KRR$^{17}$, KV$^{11}$, Kry$^{12c}$, KBMM$^{10}$, LJL$^{11}$, LWX$^{14}$, LRY$^{17}$, LYL$^{12}$, LXD$^{13}$, Lnt$^{10}$, MZB$^{13}$, MCE$^{11}$, MNV$^{17}$, MC$^{17}$, MG$^{19}$, MC$^{12}$, Men$^{10}$, MG$^{12}$, MKM$^{11}$, MS$^{14c}$, MPRCEG$^{12}$, ND$^{11}$, NFD$^{10}$, OAC$^{17}$, OPP$^{14}$, OVT$^{16}$, Owe$^{17}$, PCMG$^{12}$, PRG$^{10}$, PAK$^{15}$, RFEGP$^{16}$, RB$^{11b}$, SS$^{10}$, SVRG$^{12}$, SG$^{19}$, SGK$^{12}$, SRAS$^{16}$, SAHA$^{12}$, SLS$^{14}$, SK$^{11}$, SSP$^{17b}$, SPI$^{14}$, SHW$^{13}$, SM$^{17}$, SK$^{12b}$, SS$^{13}$, TTD$^{13}$, TMM$^{14}$, TL$^{15}$, UDVD$^{10}$, VO$^{12}$, WLS$^{19}$, WXB$^{11}$, WZW$^{17}$, WHM$^{14}$, Wu$^{11}$. complexes [YZI$^{10}$, YZL$^{11}$, YZW$^{15a}$, YYY$^{12c}$, YZZ$^{16}$, ZPR$^{10}$, ZQC$^{10}$, ZLZ$^{10}$, ZQJW$^{13}$, ZLZ$^{14}$, ZZZ$^{15}$, ZHL$^{19}$, ZSQ$^{10}$, ZFS$^{11}$, ZLWZ$^{16}$, ZSS$^{14}$, ZQXP$^{17}$, ZBB$^{17}$]. Complexity [GN$^{19}$, EMED$^{12}$, LRMAA$^{19}$, SMOD$^{11}$]. compliance [NH$^{18}$]. component [AB$^{18}$, CW$^{16}$, FZC$^{14}$, KKT$^{13}$, KKT$^{14}$, MHT$^{10}$, MM$^{19}$, SN$^{15}$]. components [LVPI$^{12a}$, NIK$^{19}$, Na$^{12}$, RL$^{12}$]. composed [TK$^{16a}$]. Composite [KO$^{10}$, ZJS$^{13}$, CC$^{19}$, Mor$^{12}$]. Composite-system [KO$^{10}$]. composites [KT$^{12b}$]. composition [GLF$^{12}$, GbZA$^{10}$, IBA$^{11}$, Ladi$^{14}$, LKN$^{13}$, QZH$^{13}$, XT$^{13}$, XT$^{14}$]. composition-dependent [LKN$^{13}$]. Compound [ZST$^{10}$, KWC$^{10}$, LLLB$^{13}$, MQA$^{17}$, PGG$^{12}$, RCM$^{19}$, SKS$^{10}$, SSW$^{16}$, TLY$^{10}$, TXL$^{10}$, WR$^{14b}$, vL$^{13}$]. compounds [AMK$^{10}$, ASD$^{18}$, BG$^{13}$, BH$^{10a}$, Buc$^{11b}$, CCA$^{12}$, CHV$^{14}$, FC$^{19}$, GZMC$^{11}$, HZG$^{12}$, KM$^{12b}$, LODB$^{13}$, LV$^{19}$, LTdS$^{10}$, LTL$^{18}$, LWJL$^{10}$, MLC$^{11}$, MPMCM$^{11}$, MW$^{16}$, Mor$^{12}$, MSR$^{11}$, OPAV$^{18}$, OG$^{19}$, Pan$^{19}$, PP$^{19a}$, PI$^{13}$, PH$^{12}$, Pie$^{11}$, PP$^{19b}$, RDM$^{11}$, RRK$^{16}$, RR$^{19}$, SMC$^{18}$, SLC$^{18}$, Shi$^{13}$, TSvL$^{16}$, TWR$^{15}$,}

[EAK$^{+10b}$, EAK$^{+10a}$, EI11, THSR13]. corrosion-inhibition [THSR13].
cosine [GH11, GE12b, LLH15]. Coulomb
[SS12, CF14, ARG11, BPL13, BBL12, Fin16b, FRGC10, Fuk12, GH11, IOO18, 
JH13, KH12, KWWH18, KK13, LLH15, Luz12, Nag16b, NDP10, PGGRMP10, 
Rit12b, Roy13, Roy16, SMOD11, Sil14, TC12, WWGW18, ZX12].
Coulomb-attenuated [NDP10]. coulomb-attenuating [CF14].
Coulomb-like [PGGRMP10]. Coulombic [Roy15, YW11b].
Coulombic-like [YW11b]. coumarin [MDNDO$^{+16}$]. coumarins 
[GTSC$^{+19}$]. Counter [XLGA12, ZLWL16, MMSC19, Oni10]. Counter-ion 
[XLGA12]. counterpoise [KPH$^{+12}$]. counting [JL12a].
Coupled [BJ12, Cam10, Cam12, Car19, PCV19, Sto18, VVVB10, 
WCC17, BVP13, BVP14, BSM$^{+15}$, CSVCB12, DMAB12, DLM12, LRP$^{+11}$, 
LP10b, Luz08, MPT11, PB10, RS12b, RSN12, SZS$^{+10}$, Sza13, Tob19, Var11, 
XDM$^{+10}$, YK13, ZE18]. Coupled-cluster
[Cam10, Cam12, PCV19, LP10b, PB10, SZS$^{+10}$, Sza13]. coupling 
[ATL$^{+14}$, Ash18, BJ12, BSV12, CCP18, CFG11, CSP$^{+10}$, CDT12, 
IROW10, Kry10, Lar10, LKOS17, LW15, MKD19, MC18b, PM12, RCP14, 
SSI$^{+10}$, Shi18, SHS$^{+13}$, WTP$^{+19}$, Wit18, YSS$^{+10}$, YH14b, ZLS$^{+18}$].
Couplings [HKLW13, Kaw15, LB19]. course [HSYM11]. covalency 
[MML11b]. covalent [ABS13, AB16a, MURR13, NE11, YLH$^{+19}$, KK13].
Covalent [MML11b]. Cover [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, 
Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, 
Ano13k, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13x, Ano13y, Ano13z].
Cover [Ano14a, Ano14b, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o].
Cover [Ano14p, Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z, Ano15c, Ano15d, Ano15e, Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15v, Ano15w, Ano15x, Ano15y, Ano15z, Ano16a, Ano16b, Ano16c, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m]. Cover 
[Ano16o, Ano16p, Ano16q, Ano16r, Ano16s, Ano16t, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16b, Ano16c, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m]. Cover 
[Ano16o, Ano16p, Ano16q, Ano16r, Ano17a, Ano17b, Ano17m, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17y, Ano17z, Ano17c, Ano17d,

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].

cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands [ELC08]. cyanuric [EMK14].
decahedral [VS19]. decanethiol [FFF10]. decapeptide [DGA+13]. decarboxylation [EAH13].
Decay [AC11, ASD14, Cao17, CCM08]. Decisive [SC18].
defects [ES17, KC19a]. deficiency [MFR10]. defined [Fin16a, Gru17].
Definition [LVP12a, Kon11, MBTVR12]. definitions [Tch16]. Deflation [MQG13]. deflection [AOLB12].
deformation [GMP+11, KK12a]. deformations [KMT+12]. deformed [Agb12, MJ11].
deglycosylation [WHS+13]. degradation [HYZ+13, SL+15, dlLIAI+12]. Degree [YIY+13, CAAII2, GV19, LSW19, LWY19, PR11b, PL18a].
degree-Kirchhoff [LSW19, LWY19, PR11b, PL18a]. dehalogenase [ZCZ+12].
dehydrogenation [HSYM11, NTNL10, WZM+13]. Delayed [SGG+10, GMM+18]. Deletion [Cin11a]. delivery [RdPW+12].
Delocalization [DZO11, LNI12, ARH+13, AT18, LDKB15, MJ16b, NE11, NRGSI11, RBVAG18, WDSL14, WWD+15]. delocalized [ALK18, DG19, Joh17]. delta [DAC11]. demon [CD15].
dense [BN12, DW12, Ng12]. densities [ALRA10, ALRAE11, BPL13, Fin15, LS17, MAT19, MT11, MNZPT19, SS19b, WGLX10, ZL12]. Density [Ano13-49, BHA19, BGBV12, BJdlMAV12, CCL+13, CM12, CD12, DCBB11, DSZB18, DQZF12, EM16, ED16, FZX18, GMR18, GGD12, HLL+14, HKLW13, HYD11, ISN13, IKN13, JS17, Kar13, KCC13, KK14b, KSIAK7, Kit14, Kit17, LACel, LWL+12, LWX+14, LBY+14, MLC+11, MW16, MUNZVR12, MIN13, MLB+12, MM13, MCRS16, MOH+12, NTNL10, NZAVR10, PS10b, PS14, PMH+16, RGPZD13, SA18, SVRGV12, SKY+13, SS13, TOSN12, Tan12, TIN13, TDOD17, TFZ+15, UMS13, VUC13, WJL+11, Wit18, YKM+15, YLI11, ZCZ+16, ZRR+11, dCSDdMC13, AC19, ABLT11, AK17, AM13b, AB18, ATM17, AGPDZ13, AST16, BMK+14, BD14, BGC12, BVCAPI2, BL19, BDF+16, BDF+18, BLdV19, BLKB11, CDSK12, CEFM12, CM15, CINSK11, CH17, CZLD17, CLH14, CC19, CK17, CF14, CC11b, CSTA16, DWJ11, DKS11, DPKR12, DW12]. density [Dil13, DZ11a, DGR+16, DG19, FO10, FDNR10, Fin16a, Fin17, FA17, ...
MLPT10, MDNDO\(^{+16}\), MBBT\(^{+12}\), NRHJ11, OAA19, PPK\(^{+13}\), QHS11, RYM12, RBZ15, RMP\(^{+14}\), SF13, SST\(^{+11}\), SRMB15, TZ11, TKS\(^{+17}\), Val17, VV18, VMC11, VHTEG15, VBO\(^{+15}\), WGLX10, WLL\(^{+13}\), WJ11, YWR\(^{+18}\), ZSAP11, ZZX10, ZZR\(^{+17}\), ZYL\(^{+13}\), ZMB\(^{+17}\), ZFC12. derived [CADSG18, MAN15, NH18, PAKA15]. describe [CB10, MMG15, PABSK16, Sza13]. describing [Gar08, JCC10, dGR14]. description [AB18, DVDBM11, DCFD10, DMBL16, Fer19, FGD\(^{+19}\), GC19, HF\(_{d}\)GC14, KQ14, LORR\(^{+12}\), MPMMC\(^{+11}\), MBA\(^{+19}\), Nas19, NGS11, SIM14, SFL\(^{+10}\), TCA10, TRZ\(^{+19}\), ZZ18]. descriptions [PC16, PCK19]. descriptor [AKR12, FDG18, PUGSFM18]. descriptors [GI10, GI11b, GI11c, GI11e, JS18, LV19, LNV\(^{+18}\), Nag16b, Nal15, OPAVM18, PH12, Pog12, TFA10].

Design [FZH\(^{+18}\), HSS18, IIS\(^{+17}\), cLqFt\(^{+14}\), Val17, BJ17, CAA19, DC14b, GbZA10, HM10b, LLZ\(^{+14}\), LZ\(^{+17}\), MY17, MSM16, Ném14, Oni12, OW18, SRASZ16, SAHAA16, Sk18, SLA12, SSS15, STM18, THL\(^{+15}\), TK16b, VV18, WWB\(^{+14}\), WR14a, WR14b, XFW\(^{+14}\), YZZH15, YHL15, ZFW14, ZWZK19]. designed [NTGC19, OAA19]. designing [SSB12a, ST15].

desorption [´AFV12, FTB11, GD11]. Dess [TM19]. destructuring [KRG\(^{+13}\)].

desulfurization [VPGC12]. detachment [DZO12c, DZO12a]. Detailed [Sch13, Fin14a]. Details [Lar10].

detachment [DI10]. Developing [AV19].

detachment [DI10]. Developing [AV19].

detachment [DI10]. Developing [AV19].
RYW⁺15, RNdA⁺10, RFMC19, RS₁₁b, Rua₁₀, SSP⁺₁₇a, SSB₁₉, SMGZF₁₉, Sat₁₁b, Sch₁₂a, SMEH₁₅, Ser₁₁a, Ser₁₁b, SAHA₁₂, SHE₁₀, SM₁₃, SS₁₈b, SB₁₀b, SBB₁₆, SHW⁺₁₃, SMGZ₁₃, SWS⁺₁₄, Tas₁₄, Tau₁₂, TGRP₁₉, TG₁₃, Tug₁₃, TKS₁₇, UV₁₈b, VF₁₃a, VV₁₈, VLG₁₂, VSN⁺₁₁, Vie₁₇, WLWT₁₂, XX₁₂, XZ₁₁, XZG⁺₁₈, YNLD₁₈, YS₁₅, YY₁₈a, YY₁₈b, YYI⁺₁₂, YIV⁺₁₃, YZL⁺₁₁, YYW⁺₁₂, YZW⁺₁₅a, YZZ₁₆, ZASP₁₁, ZLWL₁₆, ZL₁₀, ZQXP₁₇, ZLY⁺₁₄, ZPW₁₆, ZCP₁₁, ZDZL₁₁, dSdS₁₃a, dSdS₁₃b, dSM₁₉a].

DFT-based [BP₁₃, Dw₁₃, MCP₁₀]. DFT-D [BAB⁺₁₈]. DFT-D3 [SSB₁₉].

DFT-treatment [AEKGZ₁₂]. DFT/M₀₈ [Vie₁₇]. DFT/M₀₈-HX [Vie₁₇].

DFT/TB [ZCP₁₁]. DFT/TD [LGS⁺₁₆]. DFT/TD-DFT [LGS⁺₁₆].

DFT/TDDFT [BAA⁺₁₈, YZW⁺₁₅a, ZASP₁₁]. DFT/UFF [JLL₁₁].

DFTB₃ [PSC₁₅]. dG [XLGA₁₂]. di-anionic [DHYC₁₉]. di-enol [Val₁₇].

di-lanthanide [OAC₁₇]. Diabetic

[CHM⁺₁₇, ART₀₈, DMAB₁₂, DMI₂, KUY₁₆, MHOG₁₈, MKD₁₉, SHS⁺₁₃]. diacetyl [TM₁₃]. diagonalization

[GBK₁₈, Man₁₆, MBSAG₁₆a, MBSAG₁₆b]. diagonalizations [CKYR₁₈].

diagrams [FMKJ₁₄, Jen₁₃]. diamagnetic [Pit₁₂, RP₁₁a]. diamantane [BBKO₁₆]. diamines [LKOS₁₇].

diamino [LLW⁺₁₁]. diaminoanthraquinone [DKS₁₁].

diamon [GZ₁₄, ZWWY₁₀]. diamond-like [GZ₁₄]. diamions [TIN₁₃]. diarylethenes [MPJ₁₂, YXM⁺₁₈].

diastereocontrol [SFW₁₂].

diasteroselectivities [TFZ⁺₁₅]. diasteroisomers [BCF⁺₁₁]. Diatom

[CNBPRe⁺₁₅]. diatomic [Agb₁₂, BKM₁₅, BB₁₀, CP₁₃, CJOOW₁₁, GM₁₁, GS₁₁, HRT₁₂, HVR₁₈, Ish₁₄, JZP₁₇, KBGC₁₂, KBG₁₇, Leh₁₉c, LLP₁₇, MPM₁₅, NDH₁₀, RC₁₁, Roy₁₄, SY₁₆, Tou₁₁a, VOAH₁₈, Leh₁₉b].

diatomics [G₁₁b, G₁₁c, IM₁₅]. diaza [ZLS⁺₁₈]. diaza-benzo [ZLS⁺₁₈].

diazaadamantane [KMK⁺₁₆, KMM⁺₁₈]. diazadiborinine [GC₁₈].

diazine [BHA₁₉, CW₁₆]. diazo [TLT₁₈, LDW⁺₁₁]. diazonium [Bon₁₇].

diazotization [LLW⁺₁₁]. dibenzothiophene [VPGC₁₂].

dibenzoanthracene-like [VPGC₁₂]. diberane [ZYL⁺₁₄].

diborane-... [SSB₁₉].

dicarbon [FC₁₉]. dications [Buc₁₂b, GNM⁺₁₂].

dichalcogen [KM₁₉].

dichloro [LCS⁺₁₁a]. dichloro-germylene [LCS⁺₁₁a].

dichloroketene [CHH⁺₁₉].

dichloromethylbenzimidazole [PMC₁₁].

dichloropropene [ASMP₁₅].

dichlorosilylene [LLLB₁₃]. dichotomy [GTM⁺₁₈].

dichroism [PCR⁺₁₁, SB₁₀a].

diclofenac [KK₁₉].

dicopper [BH₁₀b, RNDA⁺₁₀].

dicyclobutadieno [LWY₁₉].

dielectric [CN₁₂, KPO₁₀, KT₁₂b, Ng₂, NDM⁺₁₂, OA₁₃, RTG⁺₁₉, Ser₁₁a, Ser₁₁b].

diellectron [LB₁₉].

Diels [MIK₁₉].

dien [LWS⁺₁₉].

dienes [LW₁₁, LKZ⁺₁₆].

dieniminium [BMX⁺₁₉].

diennone [KAOB₁₁].

diethyl [KI₁₅].

diethylidichalcogens [Dum₁₂].

difference [AD₁₇, Fin₁₆a, Kim₁₆, LCZ₁₅, WH₁₈]. differences [ALK₁₉, WBW⁺₁₈, BB₁₆, MK₁₀a].

Different [MAT₁₉, ABP₁₃, ABA₁₁, BS₁₆, CW₁₆, CP₁₁, FM₁₆, GI₁₁e, GGP₁₃, HGB₀₈, JdOS₁₆, KP₁₀, LZZ⁺₁₇].
MNP19, MIKH19, TW10, TFZ+15, YŞÖ12, ZCW16, Zil14]. differential
[Ali14, yBZIC18, CRA+11, HVR18, Nag10]. differentiation [CW11].
difficult [KLE+19, Mar12]. difficulties [Sut12]. diffraction [ÖEDB11].
diffuse [SZS+10, SLZ+11c, SLZ+11a]. Diffusion
[JCCZ12, PP10, ABG12, BR12b, HKZZ15, LWX+14, MFOH18, RJPGL+13,
SR19, UDS19a, WLH+19]. difluorohydroxyborane [MMCN+11]. dihydro
[SC12b, TAY11]. dihydrobenzimidazole [KKG12]. dihydrobenzoxazoles
[ZBG+19]. Dihydrogen [dOR10, AKHS13, GD11, GT13, MS14c].
dihydrolipoic [PM17]. dihydrolutidine [TM13]. dihydrobenzimidazole
[KKG12]. dihydrobenzoxazoles [ZBG+19]. Dihydrogen [dOR10, AKHS13, GD11, GT13, MS14c].
dihydropyridines [ZYSW17]. dihydropyrrolones [VGGPdL19].
dihydrothiophene [HL19]. dihydroxyacetone [BGJSM+18].
dihydroxybenzene [YY18a].

diimide [HSS18]. diiso [LKOS17].
diketonato [AC19]. diketone [SKS10].
diketone [SS13].
diketopyrrolopyrrole-analogue [PWP+18].
diketopyrrolopyrrole-thiophene [MSG16].
dilauroyl [MKSG13, TTM16].
dimetal [ZFC+17]. dimetalloocene [LYD+18].
dimethoxyphenol [Tan12].
dimethyl [JSLH14, JAB12, LdBF+12, LXLL11, NMHPGV12, Owe17, SJZL12, SSP14,
SCZH16, TAY11, TXL10, WXZ+11].
dimethyl-germylidene [TXL10].
dimethyl-silylene [LXLL11].
dimethylamine [LLZZ10].
dimethylaminophenyl [FO10].
dimethylaminophenol [WZX11].
dimethylcyclobutene [MB13].
dimethylmethylenephene [LWC+10].
dimethylnitrosamine [LdSDM14, dAVdM17].
dimethylnitrogen [VPOG19].
dinitrogen [LDW+11].
dinitrophenol [RNDA+10].
dinitrosamine [JN13].
dinuclear [FDNR10, PEA+12].
dinucleoside [PAD+10].
dinucleotide [Cys11].
dinucleotides [HW12].
dioctahedral [PDR+17].
diodes [MUNZVR12, NZAVR10].
diols [LKO17, SBEH11].
dione [OPP+14, QJ17, IC14, KDC12].
dioxabicyclo [VOK+18].
dioxane [Cai10, CNSK11].
dioxetanone [dSS13b].
dioxetanones [dSM19a].
dioxide [JLS13, KKT13, KKT14, MPL+11, PP14, TDOD17].
dioxin [MSY+12].
dioxolene [DG19].
dioxyn [KMK+16, KMM+18].
Dioxogen [MMA13].
dioxygenase [ASD18].
dioxygenation [ADR+18, ASD18].
diperfluorophenyl [WDS19].
diperoxide [SRA+11].
diphenyl [YWJ+11].
diphenylamino [CRSB12]. diphenylcarbene [GLXL18].
diphenylformazans [TT10]. diphenylpolyenes [MMWA11].
diphenylcarbene [GLXL18].
diphenylformazans [TT10]. diphenylopolyenes [MMWA11].
diphosphinito [ED16].
dipolar [BL11, DI10, ELC08, YNLD18]. dipole [AM12, Ber13a, Ber13c, BVP14, GFB12b, GI11a, GI11c, HK11, IMS+13, KA11, LK13, MA11b, MD11, MVA19, MNS11, SS12]. dipoles [SMEH15].
Dipole [AM12, Ber13, DI10, ELC08, GI11a, GI11c, HK11, IMS+13, KA11, LK13, MA11b, MD11, MVA19, MNS11, SS12].
Dirac [DJ12, Agb12, Bay19, BCNR18, DJ95, NF11, RW12, Rit12b, SS12].
directional [MMF+13, NYS+10, PCK19, Shi18, YSS+10]. Diradianology [NKF+13]. Diradicals [BSM+15, CKL16, ZLS+18].
Diradical [MMF+13, NYS+10, PCK19, Shi18, YSS+10]. Diradicalology [NKF+13].
direct-potential-fit [Haj18].
Directed [DKR10, ABS13].
directional [SMP10].
directional [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].
directed [DKR10, ABS13].
directional [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].
directed [DKR10, ABS13].
directionally [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].
directed [DKR10, ABS13].
directionally [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].
directed [DKR10, ABS13].
directionally [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].
directed [DKR10, ABS13].
directionally [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].
directed [DKR10, ABS13].
directionally [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].
directed [DKR10, ABS13].
directionally [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].
directed [DKR10, ABS13].
directionally [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].
directed [DKR10, ABS13].
directionally [SMP10].
directionally [KUTS10].
directionally [Kri13, WWL17].
direct-potential-fit [Haj18].

disarm [NP18].
discontinuously [GB10].
discotic [SSKS12, ZSASS13]. discovered [VVY18]. discovery [CAA19].
Discrete [ARH+13, CP11, FLCHL10, HHL+12b, KyH13a, LKLW11, Na12, SSdS17, TK6a, ZZZ11, Haj18, Na13, Sha11b, SGL19, VPG12, WWHZ13].
disarm [NP18].
discontinuously [GB10].
discotic [SSKS12, ZSASS13].

diselenide [Dum12].
diselenide-linked [Dum12].
dismutase [CWZ+10, PM17].
disorder [PDR+14, Wan13].
dispersing [ISRK12].
Dispersion [KKH12, SA18, Dob14, ISN13, IN15, KGOR17, LCT14, MS17, PSC15, Pit12, SKY+13, WYJ15, dCDC+11].
dispersion-corrected [MS17].
Dissociation [CK17, GM11, PW10, SSW16, SM10b, BMBD10, Bla15, CC11b, DSZB18, GSAY11, GLT13, GRLA18, GD11, KWC10, KZA+17, KT+12, KMM16, LLL16, MMBK12, MNE+13, OKR12, OK16, dMOB12, RPBB11, Rua10, SLZ+11b, SB10b, SQ10, SY14, SY16, SCS15, TJS17, VSMK13, VO11, XX12, ZZX10, ZCC11, ZSHL14, ZZC12, dSNBG08].
dissociations [TCA10].
dissociative [DLCB15, Kry12b].
dissociation [KLK13].
distance [GI11b, LSS19, SXH18].
distances [GST11].
distillation [TB15].
Distinguishing [ZR13].
distortion [CL11, YI+13].
distortions [GFB12a, GHCMMQM17, PK13b]. distributed [RAMB18].
distribution [ABP13, DPRK12, EPS+16, GGD12, LGHL11, PK13a, RCM10, SAC18, SM14a, TMM+14, WZX11, vLRRK15].
distributions [GV19, LSS19, LBdV16, SVPTM+10].
distyrylpyridine [MUPC10].
disubstituted [TTB+19, dOdONM12, dSNBG08].
disulfide [Jan10, KKT13, KKT14, WXZ+11, WHY+14, ZMB+17].
disulfides [GSAY11].
dithio [NA12, PS13a].
dithio-substituted [PS13a].
dithiolene [SDR+13, ZLZ16].
dithiols [LKOS17]. dithione [QJ13].
divalent [NFD+10].
divergence [ALRAE11, Rit12a, Rit12b].
divergence-free [Rit12a, Rit12b].
divergent [DB13a, SWS+14].
Divide [SKHN13, YKN13, SN15].
divide-and-conquer [SN15].
Divide-and-conquer-based [SKHN13, YKN13].
divided [HS11c].
divinyl [dLIA1+12].
divinylene [FO10].
division [FDG18].
Dj [Shi13].
DJ [Shi13].
DMABN [CFP+10].
DMABN-Crown4 [CFP+10].
DMABN-Crown5 [CFP+10].
DMAP [LLF17].
DMAP-catalyzed [LLF17].
DMC [RYW+15].
DMRG [MFLP12].
DMSO
dye-aggregates [WKE17]. dye-sensitized [AGJ12, FM16, cLqFtW+14, PMAP12, QJ13, SSS15, WWB+14, Zha17].
dye-sensitized dyes [AGJ12, BBM17, BM16, FBU+11, GMA+19, JPPA10, JWG+12, cLqFtW+14, MY17, Mas10, PJ10, WWB+14, ZSAP11].
dyads [MUNZVR12].
dye [AGJ12, BBM17, BM16, FBU+11, GMA+19, JPPA10, JWG+12, cLqFtW+14, MY17, Mas10, PJ10, WWB+14, ZSAP11].
dyad [BGM11, BGM12].
dyad [BG17, BGM11].
dyad [BG17].
dyad [B11, BBM17, BM16, FBU+11, GMA+19, JPPA10, JWG+12, cLqFtW+14, MY17, Mas10, PJ10, WWB+14, ZSAP11].
dyad [BGM11].
dyad [BGM12].
JLG+12, Lad14, LSR10b, LZ12, LPOP12, LWL+12, LLC+11, LWJL10, LB19, MNP19, MG12, MS10, MSK+12, MPT11, MW15, NTCG18, ND10, OKK10, OA13, PCMG12, RY12, RMTG11, RRK16, RR19, SD13a, SIM4, SM19, SAHAA16, SPI14, SK10, STU19, TYN13, TM18, TJS17, WWL+11, XTLA13, XTLA14, XWCY11, XZJ+16, YRN+11, YKN13, YD17, ZGSM15, ZKW17, dSSF16b, dSSF16a, dAVdM17, Jan10, JWG12, ZAE10].

Effective [AST19, CEM14, Liu15b, May14, TSvL+16, Vik11b, YHL+13, BCGC12, CCBR+12, Dw13, GbZA10, KUY16, MPTZ13, MZST16, PGGRMP10, TG16, ZE18, Liu16].

effectively [ABM+19].

Effects [ABA11, BS16, Bla15, CAO18, KSAK17, LLZ+12, MSRn+11, PETB18, AGOP18, ACF+11, Ali14, AEM+12, ALMY18, BHMM19, BH10a, BSO16, Chr10, CFGC11, DCD11, DPDR11, DWZZ15, DLLA10, EHKD11, EKD12, EEMSS14, EAV16, Fer11, GR11, GBS17, GWM11, GZF13, GR10, GRCATG19, HZW18, Ire12, IROW10, IK14, JA12, JHS18, KI15, KRG+13, LDKB15, LGHL11, LDW+11, MNZPT19, MZLM17, MKHM11, MURR13, MPE11, NG11, NMHPVG12, Oni10, OGvSG18, OK19, PCR+11, PWP13, QHS11, RTLAT19, RP11b, RFN+12, RS12a, RSN12, RSM12, RdA11, Ril10, SH18a, SKT15, SP19, TK16a, TV13, TFSRM11, TH12, Tob19, VFCSC17, VMK13, WDR+11, WLC+17, XX12, XLGA12, XDM+10, YZW+15a, YMY+13, YT14, YFY17, ZH12, ZLS+18, ZBG+19, ZYL+13, ZBBB17, ZFC12, dCDC+11, dSMT+18, dSNBG08, SMK+12].

Efficiency [Cal10, AGOP18, ATPRV11, BDG17, Mai14, THSR13, VRO+12].

Efficient [BL16, KI15, SHW+13, SCBP17, YM14, ZWSF16, ZRLV10, CKB+19, FZH+18, FM16, IIS+17, LCK+16, OAA19, SKLC19, SGH10, SAHAA16, WTP+19, WZX15b, ZCX+16, ZKW17, dSM19a].

EGEE [LG10].

Ehrenfest [KUY16].

eigenfunctions [PMGMGR12, PBR18].

eigenstates [KB12].

eigenvalue [Mit11c].

eigenvalues [Mit11c].

eigenvector [LHX+19].
eight [SALK19].
eight-vertex [SALK19].

Einstein [DCD11].

elastic [Per10b, UV18b].

Electric [CB19, MJ19, SS12, BL16, CHL+19, CBK18, DB15, EBR11, GM18, GV11, KA11, KT12b, LB19, MM19, PCD14, SMEH15, SMEH16, SM19, VRO+12, YSÖ12, Zha17].

electrical [GKS10].

electride [OCL+18].

electrides [HWL16].

electrocatalysis [MLW16].
electrocatalytic [FFPD16].
electrochemical [AVG19b, NBZG16].
electrochemistry [FFPD16].
electrode [KJ15, Tug13].
electrodes [Che13].
electrodynamics [FNIT16, IFT14, Lin14, Liu15b, Liu16].
electrolyte [DLO16].
electrolytes [AVG19a, MNE+13, Pha19].
electromagnetic [Bae14, NTGC19].

Electron [Bas11, DZO12c, DJ18, DSVP15, LC16, LRMAA19, LZ10, MT11, PUN+11, PI16, RNP12, RBVAG18, SLG11, VBC+12a, AA11, AOT+18, Ali14, AEM+12, AGG+18, ALRAE11, AM18, ARH+13, AST16, AT18, BLJ+13, BMHN19, Ber13a, BL10, BL11, BSSS19, BKM15, Buc10, Buc11a, CMR13, ĆW13a, CM15, CG12, CH17, CSMZ10, CSTA16, DLBL15, DAA16, DLJT14, DTEMK11, Dil13, DZO12a, DLLA10, Dum12, DSSM18, ETGLMJ+19, FYhC11, Fin15, FA17, FMMD+10, GAPK+19b, GSaY11, GTR11, GS10, HSN18, Jdl08, Jan10, Joh17, KWLS15,
Kar12c, Kha16, KPL+17, Kit15, Kri13, KM19, Kuz19, Lar10, LCH14, LZZ+11, LWY13, LYL+12, LG12, Lu10, MK18+11, MR12, MW16, MJ16b, MPD+10, MPZWD10, MGB18, MJ11, MNS11, NA14, NCMC+18, NIK19, NBZ16, NAK+17, Ng11, NG12, NDM+12, NE11, NRGS11, NMV+14).

**electron** [OAT+13, POLV12, PL11, Pir13, PNC19, RBGGM18, RNV+12, RCM10, RAGM10, RS13, RKCK19, SDS19, SS10, SBMM11, SBM16, SYK+12, SPD+18, SSAM13, SHS+13, SM12, Sit15, SL13, ScBsR+10, SBKJ18, Srl18, SP19, Tob19, TC12, VFC13a, VBC+12b, WLS+19, WWD+15, WH12, XZYS10, YNLD18, YRN+11, YHLC15, YD17, ZDZO10, ZFS+11, ZZZ+18, ZSZ14, JJS13, dA12, dCDC+11]. **Electron-density** [RBVAG18]. **electron-group** [WH12]. **electron-muon** [RAGM10]. **electron-N** [SSAM13]. **Electron-pair** [LRMAA19, MT11, WH12]. **electron-proton** [DLCB15]. **electron-rich** [YNLD18]. **electron-withdrawing** [BSSS19]. **electronegativity** [CG12, GI11b, GI11c, GI11e, GI11f, Kan18, TSBSM12]. **Electronic** [AB16b, AC19, AGB19, AVG19b, BZBZ13, Ber13b, BVP14, BBYZ18, BBAL12, BG11b, BG11c, CZL17, CJGT12, DZO12b, DLLA10, FBO+11, FMCA11, GZF13, HHCA10, IA13, KK11b, KLZQ15, KP13, LvdSm14, MLY+16, MFZ+18, MS14b, MKn11, NBL+14, NDM+12, Pup11a, RK12, RZC13, SGC13, SBB16, TNT18, TSKN12, TSH17, VSN+11, VBO+15, XTLA13, XTLA14, YW11a, YH14a, AEKGZ12, AO12a, Ale13, ART08, AST16, BVCAP12, BPVD11, BPL13, BS11, BL10, BW15, BBB16, BS12, CWL+13, Cas15, CMCN11, CW+16, CHSO13, COP16, DIOG12, DAR+11, DDY12, DD17, DWX+16, DG19, DHC11, DHYC19, DHZS11, DSH+13, DB13b, Dm15, Dy16, ETGJM1+17, Fin14b, FSK+11, GBS17, GAPK+19b, GZ10, GWM11, GB12b, GP13b, GML16, GEL18, GJ18, GB13, GMM+18, GC19, HMI+15, HTM10, HIL19, HJ13, HWWW18, HhGqZ17, IGMK11, IK18].

**electronic** [JL12a, KG17, KRR+17, KLF+11, KCK14, KJ15, KJ16a, KJ16b, KSD10, Ksk11, KYLC19, KSY+11, KFY+12, KZZ13a, KHH10, KAOB11, KM16, Kri13, KO12, KUY16, Lai11, Lef19c, LL11, LBB+19, LMZY15, LL19, LLL+17, LBV16, DVMC19, LHL+15, LZ10, Lya14, MSG16, MLC+11, MC11b, May14, MMW11, MUNZV12, MBA+13, MPZWD10, MGB18, Mill12, MS17, MKD19, MA11a, MA11b, MM Rivera10, MJ11, MB13, MPT11, MPTZ13, M113, MW15, MSR+11, MCS16, MC1b8, NS19, NA12, NIT16, NZAVR12, Ng11, PE11, PCR+11, PAKA15, PMAP12, QJ13, QCB+10, RMLPGGGH16, RS12a, RM11, RRRV19, RNC+14, RM11, Rus14, RMY+13, SRPD16, SR12, SD13a, SB10a, SLC+18, SYL+18, SLS+14, SXS+12, SLSZ13, SIS+08, SRS+17, SSTÖ11, SR11b, SZZ+12, ScBsR+10, SS16, SK12b, TYN13, TZ11, TV13, TD11, TBB+19, TFR11].

**electronic** [TRZ+19, TG13, UTNT13, Var14, VPA11, VLFG12, WWC17, WFS13, WJS+10, YZL+10, YZL+11, YZW15b, YH11b, ZQJC10, Zha10, ZLS10, ZZZ+12, ZCG+16, ZQXP17, Zho18, ZCP11, dSSF16b, dSSF16a, Bou12b, Lad14]. **electrons** [BEM12, BB10, BB10, BMB16, Dw13, Fer19, Ign11, Ign12, ISRK12, KK13, KK14a, KV19, KRY12c, Nasi19,
Nes10, QCB+10, RP11a, RPVM10, RS13, SALK19, She12, SS19b. **electrons-Nd** [BB10]. **Electronuclear** [SL13]. **electrophilic** [Buc11b, YSA+11]. **Electrophilicity** [PC13, IG11]. **Electrostatic** [HL19, NMHPVG12, TH12, TCS10, AC19, CDSK12, DPRK12, IG11, KKS+11, KRG+13, PK13a, TYN13, ZCZ+12]. **electrostatics** [BWE16]. **element** [OVT+16, SHS+13]. **elementary** [EMED+12, EMEPD15, SOF+10, Zil14]. **eleven** [DCFD10]. **ELF** [Fin14a]. **eliciting** [TPT19]. **elimination** [BLM+12, FZC14, MM19, MLB+12, Zha10]. **elliptical** [MFLK11]. **elongated** [ALHC18]. **Elongation** [KdSM+10, XLGA12]. **else** [Kry10]. **Elso** [COP16, HS15]. **elucidating** [Kaw15]. **elucidation** [MMP+18b, SBKJ18]. **elusive** [SSP14]. **elymoclavine** [RGS+13]. **embedded** [BA13, Lan10, LC19, SMV11, SRN+19, JLL11]. **Embedding** [ABS11, DB13a, QB15, AB16a, GCK+17, HJK14, SRN+19, TGRP19]. **embeddings** [AF19b]. **emeraldine** [RMTG11]. **Emergence** [LFP+19]. **Emerging** [SMMT13]. **emplaced** [BA13, Lan10, LC19, SMV11, SRN+19, JLL11]. **Encapsulations** [RR11]. **endic** [ZPW16]. **Endo** [Jal10]. **Endohedral** [JW19, ACL12, BBYZ18, GAPK+19a, HLB19, JLL+18, LYW+19, MS17, SCTW10, WLZ+12a, WSL+11, YL11]. **endohedrally** [NW12]. **endohedrals** [YK11]. **ene** [IK14, Sat11b]. **Energetic** [GB13, GAMM10, HLB19, HM11, HZZW11, Kar15, LCCH10, LL17, MTS15, SRA+11, TCSD12]. **Energetics** [MNC12, ACMRN10, CdAFS+12, CdLaSc18, DCB11, GCD13, KUTS10, PMMG+11, Puz10, QTCL10, TBA13]. **Energies** [BBK06, LBW11, SCZG12, ASHF13, AC12, Ali19a, ABA11, BVCAP12, Bla15, CFCO+10, CHH+19, DZO12c, DZO12a, EK10, FLvLA15, FYhC11, FC19, GMA+19, GM11, GFRdG11, HNH+12, HIL19, HM10b, IKN13, Kin13, KKS+11, KB19, LDKB15, LORR+12, MMM19, Mas10, MS14c, NA14, Na13, NV10, OKR12, OK16, Pea11, PBB15, SH19, SR19, SOM10, SZL+14, Tsz15, VF13a, VLF12, WWC17, WZW17, WR15, XX12, YÇO11, YWH+12c, ZZ10, ZCC11, ZZC12]. **Energy** [CC11b, FDA16, AV19, AG10b, AK17, AB18, AOLB12, AEM+12, ART08, AZD+11, AST16, ALK19, BXR+13, BPVDB11, BP13, BAP12, BSS16, BBL12, Ber13c, BVA+14, Bou12b, Bud12, CPF+11, CWW12, CBNR+11, CDS+18, CCL+16, CFV18, CLH14, CSG14, COP16, DK13, DB11, DHZ11, EMK14, Fin16a, FMMD+10, GST11, Gra08, Gra11, HR19, Han19, HJRO13, HFD11, HMI10b, HfdGC14, HM10b, HM11, HBMM11, ISN13, IK18, Jeo18, JZP17, KKH18, KyH13a, Kim16, KSN+10, KMNSP19, KMM16, KPH+12,
Kri13, Kuz19, LFF+10, LSR10b, LV12, LWWZ13, LDZG16, LG12, LDADB+15, LVP12a, LSC+18, MZB+13, MGK+11, MDC15, MCP10, MHT+08, MA12, McC13a, MOE+11, MOLF11, MIN13, MAF19, MJSC18, MGD11, MPRCEG12, MLB+10, NA12, Ném14, Ng12, NDP10, NIT16, OPAVM18, OH19, PML+11, Per18, PMEP19, Pha19, PP14.

energy [RBGGM18, RPVM10, RGTS11, RCP14, RLER10, SAS+12, SIM14, SFC16, SGL+16, SCLCPB12, SA11a, SB16, SXH18, SLZ+11b, SRS+17, SK11, SGC13, SS19b, SW16, STU19, SZ15, SYZ17, SC18, TNN16, TSL11, Tou11b, VPA11, Vik11b, Vyb08, Wag14, WKE17, WWL17, WH18, fXxBhD19, XZZ+10, YH14b, YLC17, YLYC18, ZWL18, ZS12, ZRLV10, dHLDs12, dSSF16b, dSSF16a, Yu13].

[energy-based [SK11]. energy-dependent [FMMD+10]. energy-loss [AEM+12].]

energy-aware [SK11]. energy-dependent [FMMD+10].

[energy-relevant [Wag14]. Energy-surfaces [FDA16].]

energy-efficient [RI19, WCL+17]. enhance [ZLWL16]. Enhanced [BGL+16, TZD+19, DSD18, LLZ+14, Mas14, MS14c, MPE11, SKV12, SCLCPB12, SA11a, SB16, SXH18, SLZ+11b, SRS+17, SK11, SGC13, SS19b, SW16, STU19, SZ15, SYZ17, SC18, TNN16, TSL11, Tou11b, VPA11, Vik11b, Vyb08, Wag14, WKE17, WWL17, WH18, fXxBhD19, XZZ+10, YH14b, YLC17, YLYC18, ZWL18, ZS12, ZRLV10, dHLDs12, dSSF16b, dSSF16a, Yu13].

[Enhancement [GV19, KKT13, KKT14, SJW13]. enhancements [ATPRV11]. enhancing [MZLM17, WLC+17].

enol [AZD+11, Coo12, GW18, MPGGS19, VF13b, Val17].

enol-imine [Coo12].

enols [MPGGS19].

enones [LMCZ11].

enough [MSS11].

ensemble [AM13a, Jou13, PP16].

Entangled [Xu16, EMEPD15, SK17b, Xu19].

Entanglement [Kar15, Tap15, BT15, BT17, SPM+15, XZJ+16, ZZ15, ZBK15].

Enthalpies [Mor12, dSNBG08, HZG12].

Entropic [DTPC17, LSS19, SMOD11, LRMAA19, MR18b].

Entropies [HN12, OH19].

Entropy [AZD+11, DBTA19, Gra08, Gra11, JZZH17, NTCG18, FD11, PK+16, PSGK17, St15, SDL+15, WSV10].

envelope [MMA10].

envelopes [BW15].

environment [AG10a, GC19, JCC10, TYN13, MPL+11].

Environmental [OK19, RdPW+12].

environments [AM10, Mar13, MVA19].

Enzymatic [SCB+14, BMB12].

enzyme [DPRK12, ZST+10, dSSdSGA12].

enzymes [AHC+18, WYW13].

EOM [DVP18, TD19].

EOM-CCSD [TD19].

EOMCC [DSVP15].

F'Ph [WSML16, WSML16].

epoxidation [LMCZ11, ZLY+14].

epoxide [KMS+11, KUTS10].

eQE [GCK+17].

equalization [GI11a, GI11f].

Equation [FKBG19, UV18a, Agb12, ATPRV11, Bay19, BKM15, BR10, BR16, Cam10, CW11, CW13b, Cho16, GMGRMP12, HYZS12, HYZS19, KC16, Kha16, Kri13, MNZPT19, Nag16b, NF11, PGRMP10, PV11, PV12, PMGRM15, RZ17, RW12, RA10a, VATPR11, VAT12, WC14, Zak16, ZLJ11].

equations [CRA+11, DSCO+13, Per10b, ZLE17].

equilateral [RSN12].

equilibration [Nes11].

equilibrria [Kim19].

equilibrium [KS18, LDW+11, Nal15, NB17, SXH18, TSH17, Zak16].

equivalences [ZWE12].

Equivalent [GSZ10].

era [IAK13].

Ergodicity [NE11].

Erratum [BR12a, BC16, BT17, BW13a, DJ12, FC13a, Ig12, IK10, Kar10, LSR+11, Liu16, Mat10, RB11a, RAFL8a, RS11a, TBRIS11, TBRIS12, Yur15].

error [KB19, VSS11].

errors [LNI12].

Esteemed [Sau11].

ester [HM11, SJZL12].
esterification \cite{LMG+18}. esters \cite{CGIA+12, QCW+12, WTZ+11}. estimate \cite{BBL+12}. estimated \cite{EKN+10, Kuz+19}. estimates \cite{CFW+11, CD+18, CI+14}. Estimating \cite{CCL+16, ZS+12, Bla+15}. estimation \cite{Den+19, EMK+14, KFY+12, SK+12a, VVN+16}. Estrada \cite{HIL+19}. ethanol \cite{FFF+10, HDQ+13, MOE+11, PSKV+19}. ethene \cite{Ang+10, SKTI+15, TDG+11}. ether \cite{BBL+12}. ethers \cite{QCW+12, SCZH+16, dlLIA+12}. ethoxy \cite{DPRK+12}. ethoxypyridine \cite{MCC+12}. ethyl \cite{KI+15, KDC+12}. ethyl-pyrrolidine-2 \cite{KDC+12}. ethylbenzene \cite{HWHZ+11, SSB+12b}. ethylbenzenes \cite{MOH+12}. ethylene \cite{AKC+10, DLO+16, KI+12, LCH+11, NA+14, NIK+19, KFY+12, SK+12, SCZH+16, dlLIA+12}. ethylenes \cite{YN+18}. ethylen/linear \cite{NFK+19}. ethylenes \cite{YN+18}. ethyltoluene \cite{GK+12}. ethynyl \cite{S+BAT+16}. ethynylpyridines \cite{SM+12}. ETO \cite{G+10}. ETOs \cite{AA+15}. Eu \cite{XY+18, BRBRS+11, USL+13}. Euler \cite{Nag+16b}. eV \cite{NA+14}. evaluate \cite{CJS+11, HNH+12, PBR+18}. evaluating \cite{CKL+16, GI+11d}. Evaluation \cite{GAPK+19b, GS+10, Hat+13, NFA+12, Sch+12a, dWL+14, AA+15, BL+16, GTR+11, GI+10, HGI+11g, IGI+11a, JGI+11, JS+17, R+19, SPO+11, TPD+12, YZ+13, ZRL+10, GHI+11b, MCI+18a, OCG+19}. event \cite{GI+11a}. events \cite{CSS+16}. evidence \cite{HV+11, HHY+18, WTW+15}. evidences \cite{CG+12}. evolution \cite{ABM+19, BL+11, IFT+13, IFT+14, JL+12b, MLW+16, RGR+12, YSS+10, YSK+12}. Evolutionary \cite{CGG+18}. evolving \cite{LSR+13, VIK+11b, YY+13}. Ex \cite{NCM+18}. Exact \cite{GZSMFN+16, HR+12, HFZ+12, Kha+16, KUY+16, RBD+10, RS+13, Zak+16, AM+13b, Eng+16, FA+17, Hog+13, HII+10, Kry+12c, LEU+11, MP+11, PT+13, SFL+10, Tou+11a, FLCH+10}. exact-exchange \cite{SFL+10}. Exactly \cite{GMGR+12, PGR+10, PMGM+12}. EXAFS \cite{LSR+13}. examination \cite{Kan+17}. examine \cite{KJ+14}. example \cite{CP+10, DMB+16, MSAB+19, RB+19}. examples \cite{DL+12, Hop+15, JA+12, Mail+14, MMP+18b, Sic+16}. ExCage \cite{DI+18}. excellence \cite{MEF+15}. exceptional \cite{LA+11}. Excess \cite{BH+19, Jdl+08, KM+19, YHLC+15}. Exchange \cite{Dw+13, Fin+16a, PTH+11, ATL+14, AM+13b, Ali+19b, AGPD+13, AK+11, BHV+11, BVR+10, CWW+12, Eng+16, FB+17, IHG+10, KMK+16, KMM+18, Kry+12c, LZF+13, LCT+14, Lui+15, MMM+16, MEEA+13, Mys+12, PDR+14, RPV+10, RFEG+16, RLER+10, SPT+15, SFL+10, SFC+16, Sh+18, TAI+10, XZL+12, MRS+15]. exchange-correlation \cite{AGPD+13, AK+11, LCT+14, RPV+10, SFC+16, TAI+10}. exchanged \cite{PV+10, UMS+13}. excimers \cite{Cas+15}. exciplex \cite{KB+19}. Excitation \cite{Ky+13a, BVCAP+12, BSS+16, FMCA+11, dDGN+10, GMA+19, IHG+10, LW+13, LOR+12, Mas+10, MIN+13, SZL+14, WSC+11, YHI+4b, ZGSM+15]. excitations \cite{CD+15, VAT+12, VBC+12b, Zho+18, ZB+18}. Excited \cite{Cha+11, Glu+13, ACF+11, Ali+19b, Cam+10, Cao+17, CHM+14, CM+16, CL+18, Cor+16, DSSM+18, GWHH+17, HMA+18, IG+11k, JA+12, KTI+12a, KKI+14b, KKT+13, KKT+14, LSL+08, LV+16, LP+10b, LGZ+15, LZ+10, MMWA+11, MT+11, MNS+11, MB+12, Nes+11, NDP+10, Nic+11, PRPU+13, PMAP+12, SBD+16, SR+11b, MV+16].

F [yBZFC18, CS18, DPDR11, DSSM18, DSSM19, EMSB15, GWM11, GKT+12, GB13, HNBG15, JLG+12, KAR12a, KMM16, Kuz19, JLL+11, LGHL11, LZZ+11, LMZ+11, LLG+12, LC16, MEEA+13, PP14, RTTAT19, SB18, SKS10, SPI14, SYQ+10, SZLI+14, TMC18, TL15, WZW17, XZL+12, MLPT10, YZLW+15a, BLWJ17, DMAB12, DZO11, GKT+12, LGHL11, Ma14, MGB18, Pup11b, Sik18, SZ15, TNN16, YGL+11, ZHL+19, ZCG10]. F12 [BL12, yOITn15]. Fabricio [COP16]. fac [AC19]. face [DMWY11, DLMG12]. Factor [Tri14, Kan17]. factors [AGB19, BMX+19, Mam13, MK11, SPO+11, TZ11, VLG12]. families [GN19]. family [OOI+19, WZX15b]. Fan [Roy14]. far [Var14]. FARMS
Fast
[GFRdG11, PMHM19, PT13, PSC15, SAS+12, SLS+19, UDS19b]. Fatigue
[YXM+18]. fayalite [NDM+12]. FCu [ALMY18]. FCX [SZL+14]. Fe
[DMG10, ESS13, FTA11, MPD+10, MG10, MG16, PAKA15, Qu13, YL11,
Zha10, AM10, BGD14, BAA+18, CRB+12, DSI11, DCG10, KSD10,
LVdSD14, NKT19, OGVg18, SSP+17b, ZSQ+10, ZSHL16]. Fe/C/S
[OGvSG18], Fe/C/S-doped [OGvSG18]. feasibility [JS17]. features
[CD12, DLG12, Pie12, Sch10b, TC10]. FeCp [ALMY18]. FCX [SZL+
14]. Fe Fe/C/S [OGvSG18]. Fe/C/S-doped [OGvSG18]. females
[MEF+15]. FemEx [MEF+15]. FeFe [BGFD14, BAA+18]. female
[MEF+15]. FemEx [MEF+15]. femtosecond [HYH+10, MPC10]. Fenna
[BSS16, MSBF18]. Fermi [ABLT11, CP13, FA17, IROW10, KCD15, KK13].
fermion [FY1C11, Lun13a, Lun13b, Tou13]. Fermionics [Kle11].
Fernando [COP16]. ferrimagnet [TD11]. ferrocene [DAA16, XCY15].
Ferrocenyl [MMW19]. ferrocenium [DAA16]. Ferrocenyl [MMW19].
ferroelectric [DMS+10, DLM+11, OCB+10]. ferromagnetic [BXR+13].
Feshbach [WB17]. Fe — [SBSD18]. Festschrift [KN15]. few [Mai14, SLS+
19]. FF [LGW11]. fiber [KFY+12]. fictitious [MVA19]. Fidelity
[BCN18, CKYR18, Lur11b]. Field
[CKB+19, Bae14, BBP+12b, Bra10, BSO11, BN11, CL11, CHL+19, DCD11,
DB15, EBR11, FKL+12, Fri12, FSST16, GFZ13, GRD11, HSS+11, ISN13,
KKH18, KSC15, KV19, Kt14, KC19b, LAc14, LB14b, LB19, MM19, Mit11b,
ML+11, MJ19, NTG19, PVC12, PL11, PCR+11, Pop15, RP11a,
SRPD16, SY10, SME16, SAHAA16, SS19b, SR11b, SV11, SHMR11,
TSV+16, Vik11a, Vik11b, Vik13, Zha17, dAB17]. field-effect [SAHAA16].
field-emission [BSO11]. Field-programmable [KB+19].
field-theoretical [Fri12]. fields [Bae14, BSS16, FT13, GV11, HEVMSA+
19, KT12b, PM12, SRPD16, SME15, St18, WYM15]. file [RAMB18]. Filho
[COP16, HSS15]. film [JK12]. films [GDM+10]. filter
[Man16, MBSAG16a, MBSAG16b]. Filtered [MPV+11]. Finding
[JHL+18, SRMB15, KB12]. Fine [RDB18, RAFF18b, SCZG12, RAFF18a].
fingerprint [vLRRK15]. finite [CS17, FKL+12, NS10b, PE11, TLC+17].
finiteness [PE11]. firefly [CYLL11]. Firsova [AOLB12]. First
[BXR+13, DWX+16, FTB11, Fra17, Jia15, Kan17, KKL13, LLI16,
ILBqD+19, LJK15, MBKH19, Per10b, RZG12, RJLP+13, RRB12, TAZ11,
Wan13, WLL+19, ZWCL12, vL13, AFA13, AGG+18, BZBZ13, Bon17,
CEFMK12, CC11a, CWW+16, CJOW11, FSB16, FT15, GXZ+14, HMA+19,
IGMK11, JTMP19, KSS12, Kim13, LLM13, LBVD16, LSCSFC19, MKM11,
MJ19, Pan19, PP19a, RD14, RVO+14, TCCI10, TWR15, VAO12, VDG13,
XWCL11, XCD18, YHL+13, dWLC14, WZC+12]. first-principle [TCCI0].
First-principles [BXR+13, Fra17, Jia15, Kan17, ILBqD+19, LJK15,
MBKH19, Per10b, RJLP+13, RRB12, Wan13, WLL+19, WZCL12,
AGG+18, Bon17, CC11a, CWW+16, CJOW11, HMA+19, Kim13, LLM13,
LSCSFC19, MJ19, Pan19, PP19a, XCD18, YHL+13, WZC+12]. first-row
[CAPL12, DP11, Fin17, KUY16, PD11, SK17b, ZLE17], formyl [KSAK17], formylformamide [NJA+12]. forward [FCC11]. Foster [Cin11b].


Free [AG10b, LCG12, MLB+10, AK17, BDG17, CFOC+10, ENV15, Esr18, FM16, Fin17, FA17, GAI19, Kle11, KDA+11, LSR10b, LSG+14, Luz11a, Luz12, LGS+16, MR18b, Nag15, RCM+19, Rit12a, Rit12b, SX15, TPT+13, ZBG+19]. free-radical [LSG+14, RCM+19]. frequencies [AF19a, MCE11, RDB18, Rud12, SBAT16, SZL+14, WHY+14, YWH+12c]. frequency [HH18, MPC10, TU10, ZPZ15, ZLE17]. FRgXF [LWL19]. friendly [Sau11]. friendly [MDC15]. fringes [YS13].

Frontiers [ABA11, LSR+11, YZZH15, LSR+10a]. Fullerene-buckycatcher [DI15]. fullerene-derived [PAKA15]. fullerenes [ARH+13, BBYZ18, DI11, Den19, GZW16, JLL+18, LBW11, DVMC19, MNS11, MC18a, YLZ+17, ZCG+16, ZCTG18]. fulleroid [Iku17]. Fully [Leh19a, Leh19b, RRT10, AC12, Leh19c, RVNP12]. fulvene [HMA+18, Val17]. Function [Kut13, NS13, TKN13, TH13, YKN13, AB16a, AV19, AÔ2b, AOT+18, AOLB12, BL10, BL11, Gao11, Han19, KL11, Kub12, Liu15a, MGB18, MRS15, Ng12, OAT+13, PUGSF18, RZ17, SGT10, Sta10, SS12, SD13c, Tol19, Tou11a, UYN+13, WWL17]. function-based [AV19]. Functional [Aso13-49, BHA19, HKLW13, ISN13, IK13, MIN13, SKY+13, TK16b, AC19, AK17, AM13b, AB18, AGPDZ13, BMK+14, BD14, BCGC12, BVCAP12, BDF+16, BDF+18, BGBV12, BLKB11, BjdMAY12, CCL+13, CNSK11, CH17, CM12, CZLD17, CC19, CK17, CF14, CTDOLA10, CSTA16, CD12, DWJZ11, DCBB11, DKS11, DW12, DZ11a, DGR+16, DG19, DSZB18,
DQZF12, ED16, FCS13a, FCS13b, FZX18, FO10, FDNR10, Fin17, FA17, FSB16, GFPAV19, GCK+17, GMR18, GM11, GGD12, GHCMCMQ17, GD11, GCZ+14, HMA+19, HR19, HHCA10, HLZ+14, HZZ+19, HMH10a, HMH10b, HKHI13, HYD11, HZZW11, IN15, JR12, JPP+11, JA12, JS17, JW18, KME+18, Kar13, KPCV18, KKL+16, KSAK17, KLYC19, KSG+12, KJ14, Kri13, Kry12c, KG08, KMU+13, Lat13, LPO+12, LSR10b, Leh19a, Leh19b, LW11, LWL+12, LWX+14, LBY+14, LLW+11, LCK+16, functional [LDZG16, LLZ+12, LSC+18, LNI12, MYZ+10, MLW+14, MJ16a, MLC+11, MFK+12, MA10, MW16, MUNZVR12, MG12, MKSG13, MLK17, MLB+12, MBBT+12, MM13, MKW11, MJM19, MCRS16, MOH+12, Nag15, Nag17, NH18, NDP10, NTNL10, NL11, NMP14, NMSR14, NDM+12, NDAV10, OD16, POLV12, PSI10b, PSI14, PI13, PMH+16, PABSK16, PP16, PTH11, PR10b, Pir13, PU14, PJP10, PMAP12, PI16, PC13, QHS11, RGPZD13, RS12b, RCM+19, RPVM10, RMB18, Rud12, RCS10, SB18, SA18, SGL+16, SVRGV12, SLC+18, SN12, SAHG11, SHL+13, SJJ+18, SIS+08, SDM+12, SRMB15, Srl19, SK12b, SS13, TOSN12, Tan12, TIN13, Tan13, TDOD17, TFZ+15, TLC+17, UV18a, UMS13, VPGC12, Ven12, VUC13, Vi13, VBO+15, WKE17, WJL+11, WW11, WJY15, WD+17, WZ+11, WR15, Wit18, XNL+14, XSLF12, XGH+18b, YLH+19, YWH12a, YWH12b. functional [Yu13, YL11, ZT13, ZKKR11, ZQCJ10, ZBG+19, ZRR+11, ZMZ13, ZCG+16, ZSZ14, ZZ18, Zo18, dCSDdMC13]. functionality [ATS+11]. Functionalization [ZWWY10, JNY17, YLH+19]. functionalized [LRKM10, MSOV13, MLW16, OD16, Pli18, SPPT15, TDOD17, WLZ+12b, ZK12, ZBG+19]. functionals [AF16, Ali19b, AK11, DCDD10, DCFD10, Fin16a, HFDGC14, Jan13, Jou13, KGOR17, Lae14, LCT14, LSP+16, LORR+12, Lu15, MXC18, PSM16, PRFR17, SFC16, SMOD11, SOF+10, SSP+17b, SGC13, SX15, T10, TCA10, UV18b, VSL+15, VF16, YFY17, dSDS13a]. Functions [GLT13, IA13, KBB+13, ONK+13, CSZM10, CML+16, FRGC10, GBK18, GBS17, GTR11, GN19, GS10, HITU16, HGB08, Hog13, Hor13, KH10, Kar13, MPV+11, MSNP18, MJ11, NS13, NDLC19, Ort13, OH19, PABSK16, RZS18, SPO+11, SZS+10, SLZ+11c, SLZ+11a, SKL10, VSL+15, WH12, YM14, vLRRK15]. Fundamental [Bri13, Hor13, IFT13, MSH13, Mar13, YK13, ZJS13, Bl15, CK13, GI11b, GI11c, GI11e, VVVB10, VV12, VV13]. fungal [VGS10]. furoic [GIO12]. Further [Jor18, ZLWL16]. furylfulgide [LZZ+17]. furylfulgimide [LZZ+17]. fused [RT11, RDS19, Yaml11]. future [BJ17, MGN14, Sic16]. fuzziness [Tch16].

halogen-bonds [JLZ+17], halogen-hydride [BLL+13], halogen-oxygen [dOdCMudALR11], halogen-substituted [CLXZ12], halogenabenzene [WLZ18], halogenated [GHS12, LLW+12, TL15], halogen-… [LDZG16], halomethanes [HLJZ11], halonitrenes [SYL+18], halopyridinium [ZLWZ16], HAlS [LPG+12], Hamiltonian [Bra10, FYhC11, IM15, Kry12c, Mos14, SPAS11, SA11a, SKG11, TD11, TSvL+16, YYY+12], Hamiltonians [Li16, Cal10, CCR+12, Liu14, Liu15b, MQA17, SR12, ZE18], Hammett [DNCKCS+12], having [BB10, KP10, RNV+12, SALK19, SN11], HB [XZZ+10], HBeN [LCL+10b], HBr [LGW11, SLS+11, WZHZ13], HCN [JLG+12, Tap15], HCN/CNH [Tap15], HCNO [MKW11], HCNS [KZZ13a], HCO [WB17, WZC+12, YL10], HCOOH [XDM+10], HCu [ALMY18], HD [ZGSM15, GWZ+14a, GWHH17, Kan11, SZ15], HDCH [SZY17], H… [DB15, MNV+17], heating [ES17], Heat [MMP11, FUE+12, GVPCK10], Heats [PP19b, ZZX10], heavier [ALB18, YD17], heavy [BRM19, ND10, RRK16, RR19], HeH [NWQX11, OPC17, Vik13], HeI [DTVP+12], Heisenberg [ATL+14], Heitler [CC12], helical [MCE11, NRI15], Helium [Var11, AC11, CS13, HMP+11, Ig11n, Ig12n, KH10, KWWH18, KT12a, LLH15, OH19, Pop19, SXH18, YČ11], Helium-fullerene [Var11], helium-like [KWWH18, YČ11], helix [PAD+10], Helmolz [Koc13b], hemagglutinin [KRH13], heme [LVdSM14, LDMDCA+12, SBSD18], hemerythrin [TYN13], hemispherands [SHE10], heptagon [SCTW10], heptagon-containing [SCTW10], herbicides [CRB+12], Hermitean [Br12], heroin [RCM10], Hess [SN15], hetaryl [MMW19], hetarylazo [ČS13], heteroaromatic [VVQG17], heteroatom [GAPK+19a], heteroatom-centered [GAPK+19a], heterocycles [VOK+18], heterocycles-6 [VOK+18], heterocyclic [ABTW14, CYL+19, CDL+19, GZ14, HZZ+19, LWJL10, LZD+11, LLLB13, MAN15, Pan16, WLL19], heterogeneous [Lya19, MCRS16, PCV19, PIS18], heterojunction [OKK10, WCL+17], heterojunctions [IMS+13], heteroleptic [SK12b], heterolytic [GWM11], heteronuclear [GII11b, GI11c, LYD+18], heteropentamers [MOE+11], heteropolycyclic [TXL10], heteroporphyrins [RBZ15], heterostructures [MFZ+18], hex [Sat11b].
hex-2-ene [Sat11b]. hexaaazaisowurtzitane [DGR+16].
hexaaazaisowurtzitane/nitroguanidine [DGR+16]. hexacarbalane
[ALK18]. hexafluoroacetylacetone [DARAV12].
hexafluorocyclohexane [HWWW18]. hexagonal
[KCH19a, LPF+19, NBL+14, PL18a, UV18a, UV18b]. hexahydro [MJ11].
hexahydro-1 [MJ11]. hexanal [BCS+12]. hexanuclear
[PAPCM+16]. HF [GKT+12, LGW11, SPI14, YGL+11, YZ10, AFM+10, SYY16, SCZH16, Bou12a]. HFC [Tas14]. HFC-32 [Tas14]. HFE [KAR12a]. HFE-161 [KAR12a]. Hf
[BLKB11]. Hg [NFQ+11, WHM14]. HgClOH [RSM12].
HGGGW [MRT11]. HH [Che12]. HI [LGW11]. hidden [YLZ+17].
Hierarchy [ZLE17, PC13]. HIF [MGK+12]. HIF-1 [MGK+12]. High
[DNun15, Kin13, MPRB+10, ZCG10, Beh15, BHH+13, CKB+19, CRFR11, CLH14, CKYR18, CML+16, DBTA19, DSFT17, DSSM18, Fer11, HSN18, Jeo18, JW19, KG17, KMU+13, LCL+10a, cLqFtW+14, LMC19, Luz08, Lya19, Mai14, MDC15, Mii12, NKKN15, RGTS11, RNE10, SSP+17b, SZL+14, WCGD12, fXxBd19, ZZ+10, XCD18, YYY+12, YZ13, YM14].
high- [Fer11]. high-density [JW19]. high-dimensional [Beh15, DBTA19].
high-efficiency [Mai14]. high-energy [CLH14, ZZ+10].
high-energy-density [Jeo18, fXxBd19]. high-harmonic [CML+16].
high-level [LCL+10a, RNE10, SZL+14]. High-lying [ZCG10, DSSM18].
high-order [Luz08]. high-performance
[BHH+13, CKB+19, cLqFtW+14, Lya19, NKKN15]. High-precision [Kin13].
high-pressure [KMU+13]. high-resolution [DSFT17]. High-spin
[MPRB+10]. High-temperature [DNun15, WCGD12]. high-throughput
[CRFR11, KG17]. high-valent [YYY+12]. higher [LBW11, SMRK18].
highest [SM14b]. Highly [KPH+12, KS18, WZW17, EM19, KRRH13, LLZaH14, NDH10, OK16, OAA19, SMEH16, YAF+15]. hill [SSB12a, RA10a].
Hillman [ZQW+17]. hindered [SBEH11]. Hirsch [MC18a]. Hirschfelder
[Haj18]. Hirschfelder-long-range [Haj18]. histidine [NHG+12]. histone
d[DSMPRSF18]. Historical [Hop15]. hitting [PR11a]. HIV
HMgH [WLL11]. HMgO [LGP+12]. HMH [BL+13]. HMX
[Jeo18, LZZ+13]. HMX/NT0 [LZZ+13]. HNB [LCL+11]. HNBe
[LCL+10b]. HNCH [XDM+10]. HNgBeF [SMC18]. HNO [BL11, YL10].
HOAI [LGP+11]. HOCl [RNE10]. Hoff [Buc10]. HOH [SW12].
Hohenberg [LB14b, Lev10]. holding [NIK19]. hole
[ATPRV11, ABLT11, FV11, JLG+12, MCL11, SC18, VATPR11, VAT12, WTP+19, WLC+17, ZHL+19]. hole-transporting [MCL11]. holes [CP13].
hollow [MCL18a, PAKA15]. hollow-caged [PAKA15]. Holstein [DTFK15].
HOMg [LGP+12]. HOMO [MA12]. homodesmotic [MMM19].
Homonuclear [ZS12]. homogeneous
[CSTA16, Lak10, MLB+12, MMM+12, Sic16, Yak10]. Homology
[PTD+12, SLS+10, CSVCB12]. homolytic [KZA+17, OKR12, OK16].
Homonuclear [EMS16, KBGC12, NZ13, SZZ+19, SM14a]. HONPAS
VSMK13, WLS+19, WCGD12, WWHZ13, WWHZ13, WWLZ17, WJ11, WH18, XDM+10, YW11a, YWH12a, YWH12b, YRN+11, YWH+12c, ZAE10, ZZL+11, ZLZ+14, ZL10, dSCC12, dSSF16b, dSSF16a, dFR15b, dAVdM17, dOR10.

**hydrogen-bond** [OHDA13, SCL19]. **Hydrogen-bonded** [SGK12, CdLDcS18, CCP18, KS18, LJW+11, MT10, OA13, RNE10, ZLZ+14, dSCC12]. **hydrogen-bonding** [DB15]. **hydrogen-like** [SS12]. **hydrogenase** [BGFD14, BAA+18, MG10, DMG10]. **hydrogenated** [IIW+11]. **hydrogenation** [TGA+11, VPGC12, XSLF12, ZZC15]. **hydrogenic** [DLRMFY10, DBTA19]. **hydrolysis** [CCL+10, DSZB18, KFS13, PRFR17, PMC11, RNdA+10, YTY19]. **Hydronium** [DE18]. **hydrophobic** [NHG+12, SMK+12]. **hydroxyl** [TAY11, YLW+13]. **hydroxyacetone** [SSdS17]. **hydroxyanthraquinone** [JB11]. **hydroxybenzaldehydes** [EKN10]. **hydroxybenzenes** [ATM17, KM12a]. **hydroxybenzylamine** [AFC+10]. **hydroxcarbene** [Buc12b]. **hydroxcarnonyls** [SSdS17]. **hydroxycinnamoyl** [MLW+14]. **hydroxycinnamoyl-CoA** [MLW+14]. **hydroxyfullerene** [KK11c]. **Hydroxyl** [TWHZ14, CGIAI12, FNBK17, Ril10, XNL+14, YM13, YY18a, ZC12]. **hydroxyl-thiourea** [LCM+11]. **hydroxylapatite** [UV18a, UV18b]. **hydroxylated** [MDNDO+16]. **hydroxylations** [SSI+10]. **hydroxybutyloxy** [RS11b]. **hydroxybutyryl** [MFR10]. **hydroxymatairesinol** [SBEH11]. **hydroxymethyl** [KAOB11]. **hydroxyphenalenone** [OA13]. **hydroxypropanal** [SSdS17]. **hydroxyquinoline** [CHV14]. **Hylleraaas** [OH19, PSGK17]. **Hyper** [LDW+12, DW12, FKL+12, KP11, Kha16, Mar12, XWCY11]. **hyper-netted-chain** [DW12]. **hyper-radial** [Kha16]. **hyperbolic** [AY15, GE12b, SDL+15, dAB17]. **hyperbolic-type** [AY15]. **hyperbolical** [WC14]. **hyperconjugative** [CSP+10]. **hyperfine** [Bou11, Bou12a, Kin13, Wit18]. **hypergeometric** [PMMGGR12]. **hyperpolarizabilities** [AK11, CEFMK12, NKF+13, OCL+18, YMY+13, dWLC14]. **hyperpolarizability** [BHMM19, FSB16, GXZ+14, Kar12b, Mar11, RVO+14, WWL+11]. **hyperspherical** [BAP12, PML+11, RPBB11]. **hypersurfaces** [PBM10]. **hypervirial** [ATPRV11, VATPR11, VAT12]. **hypochlorous** [TV13]. **hypoelectronic** [SALK19].

**I-converting** [dSSdSGA12]. **i-motifs** [KUS19]. **IB** [DWX+16]. **ibuprofen** [XLN+14]. **ice** [Mil12, Wan13]. **ices** [LRP+11]. **ICN** [BBMD10, McCI3a]. **iconicity** [Tch16]. **icosahedral** [DVMC19, SR12, XCY15]. **icosahedron** [SLZ+12]. **icosahedron-based** [SLZ+12]. **identical** [XLZ+12]. **identifies** [ST15]. **identify** [MVG18].
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Identifying [BB16]. identities [Cin11a, Cin11b]. Identity
[RDB19, Buc10, Buc11a, GI11b, GI11c]. IEO [FYhC11]. IEPOX [KZZ13b].
II [Bal16, DSD18, DCdG10, FBD+ 13, LYW11, LGW11, LGS+ 16, MGK19,
NNSN17, NFQ+ 11, OAA19, RNdA+ 10, SLC+ 18, SG19, TFA10, WHM14,
WRW+ 18, YZL+ 10, ZSASS13, ZLLS10, dCSDdMC13, dARAV12, dCDC+ 11,
ADR+ 18, Bou11, Bou12a, Cam10, CPF12, Ire12, Jør18, Kry12b, Leh19b,
LSR+ 13, MS12, OH13, PD11, PEA+ 12, PVS12, QD10, SGL19, YYI+ 13,
YIY+ 13, YSK+ 12, YWR+ 18]. IIB [Eng16]. III
[CADSG18, EG10, LVdSdM14, MSOV13, MMSC19, PCD14, RMP+ 14,
SLS+ 14, SSP+ 17b, SHW+ 13, WXB+ 11, ZQCJ10, ZQJW13, ZYSW17,
ZSQ+ 10, AC19, AMK10, Cam12, CWS15, LYR+ 17, NMS+ 10]. IIIA [Eng16].
Ill [Gru17, BMB12]. Ill-defined [Gru17]. ill-posed [BMB12]. illustration
[LP10b, MHOG18, ZSZ14, RBD+ 10]. illustrative [Mai14]. Image
[Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h,
Ano13k, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w,
Ano13a, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i,
Ano13j, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13x, Ano13-35,
Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31,
Ano13-32, Ano13-33, Ano13-34, Ano13-36, Ano13-37, Ano13-38, Ano13-39,
Ano13-40, Ano14a, Ano14b, Ano14n, Ano14t, Ano14u, Ano14v, Ano14w,
Ano14x, Ano14y, Ano14z, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g,
Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14o, Ano14p,
Ano14q, Ano14r, Ano14s, Ano14-27, Ano14-37, Ano14-43]. Image
[Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-48, Ano14-28, Ano14-29,
Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14-35, Ano14-36,
Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano15a, Ano15b,
Ano15c, Ano15d, Ano15e, Ano15t, Ano15x, Ano15y, Ano15z, Ano15-27,
Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n,
Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15u, Ano15v, Ano15w,
Ano16a, Ano16s, Ano16t, Ano16n, Ano16u, Ano16v, Ano16w, Ano16x,
Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16b, Ano16c, Ano16d, Ano16e,
Ano16f, Ano16g, Ano16h, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m, Ano16o,
Ano16p, Ano16q, Ano16r, Ano17a, Ano17b, Ano17m]. Image
[Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17y, Ano17z,
Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k,
Ano17l, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano18a, Ano18r, Ano18s,
Ano18t, Ano18b, Ano18o, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y, Ano18z,
Ano18-27, Ano18-28, Ano18-29, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g,
Ano18h, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18p, Ano18q,
Ano19a, Ano19t, Ano19b, Ano19c, Ano19d, Ano19o, Ano19u, Ano19v, Ano19w,
Ano19x, Ano19y, Ano19z, Ano19-27, Ano19e, Ano19f, Ano19g, Ano19h, Ano19i,
Ano19j, Ano19k, Ano19l, Ano19m, Ano19n, Ano19p, Ano19q, Ano19r, Ano19s].



insight [LV12]. insertion [DPDR11, RRVJ10, SMC18]. Insight [DMWY11, HFL+17, She12, She13, TFZ+15, WLL+13, BGMD15, DGR+16, EM17, KCDC15, MNV+17, MC17, MMSC19, RNDA+10, SAG13, SACA18, SC11, VHTEG15, YWJ+11, AF16, Tan13]. Insights [KRH13, LWL19]. insertion [DPDR11, RRVJ10, SMC18]. Insights [DMWY11, HFL+17, She12, She13, TFZ+15, WLL+13, BGMD15, DGR+16, EM17, KCDC15, MNV+17, MC17, MMSC19, RNDA+10, SAG13, SACA18, SC11, VHTEG15, YWJ+11, AF16, Tan13].


Interaction [ASHF13, DWPK14, EG10, JLS13, MYZ+10, MRT11, RNB+10, SPD+18, SK11, TBRIS10, ZT13, Ali19b, Bae14, BLL+13, Bas11, BEM11, Ber13b, CAZ+11, CLL+13, CGM12, CGG18, CRSB12, Cha10, CC11a, CYL+18, CP16, DC14a, DVDBM11, DTVP+12, DLG12, DWZZ15, ELC08, Eng16, EBH11, EAV16, FZX18, GWZ+14b, GD11, HFD11, HM10b, JFT13, JH15, JLG+12, KMM+18, KV19, KPH+12, LLG+12, LBV16, Luz08, MMR+10, Mar12, MMC+19, NL11, NV10, NFQ+11, OA12, PSK+16, PBR18, RMY12, RFN+12, RFMC19, RS11b, RRC11, SBB19, SA18, SD13a, SD16b, SHKN13, SYL+18, Sha11b, SLZ+11c, SS11, SM14d, SWS12, SZZ+14, SY16, SCZH16, TK16b, TG16, VHTEG15, VVVB10, WLL11, WZ17, WWQ17, WG18, Win10, XXhX+13, ZST+10, ZCZ+12, ZS12, ZMB+17, TBRIS11, TBRIS12, YL10].

Interactions [KMM17, MFK+12, dCdc+11, AGRI+12, BMR+13, BAP12, BMRM19, BLWJ17, BDG17, BLdV19, BWE16, Buc12b, CNBPR+11, CdLdSC18, CNSK11, CCS13, CKL16, Chu12, CSP+10, Cyx11, DJB10, Dob14, DLP17, EAA17, EA12, EMS16, FNBK17, FRGC10, FKC12, HCH+18, HMA+19, HYD11, Jai10, JEA13, JLG+17, KdpNNS16, KMK+16, KP12, KKG12, Kry12a, Kuy10, Kuz19, LMZ+11, LC16, LYW+19, LZZ+13, LDZG16, LB18, MBZ+13, MHZ18, MS12, MIKH19, MSNP18, MPD+10, MPZWD10, MS10, MSY+12, MZLM17, MAW+18, MRR13, MMSC19, NH18, Nai13, NRI15, OA13, PML+11, PABS16, PPI6, Pie12, PETB18, RK14, Ril10, Riv11, RGR12, SB18, Sch15, SM13, SM14b, SM14c, SS13, TH12, TDOD17, TCS10, Var11, VBC+12b, VSMK15, Yak11, YJ17, Yu13,
YF16, YFY17, Zak13, ZRY+13, ZFS+11, ZLWZ16, dCSDdMC13.


interleukin [WLL+13]. interleukin-2 [WLL+13]. Intermediate

intermetallic [AO12a]. Intermolecular [EAA17, LZZ+13, MZB+13, Pie12, Yu13, ZRY+13, BPG+10, Buc12b, EML+11, EA12, KMNSP19, MB15, OA13, OD12, PML+11, SPL14, TNN16, Tav12]. Internal

[MP10, DDF+12, NH18, Sch15]. International


[MQA17]. Interpolation [RP16, DTVP+12]. Interpretation

[CFP+10, Kar12c, Mor13, DHZS11, DSH+13, MAW+18, ZPM10]. interpreted [Nes11]. Interpreting


[LKd+16, MGG15, RJY11]. intra [EML+11]. Intramolecular

[BMR+13, IJY+10, RJA+10, AV19, Buc12b, CNBPR+11, COdF+11, CKL16, EKN10, FSBA12, HNH+12, JN13, JS17, KMM+18, KSAK17, KAOB11, Kry10, LXW+12, MK11, MK12, MB15, MSBF18, NRGS11, NRP+11, NRHJ11, Tav11, Tav12, UTTn13, YRN+11, ZZ18, dSM19a]. Intriguing

[LB19, WSML16, ZLS+18, YHLC15]. Intrinsic

[Lai11, MHO+15, NH18, GJI18]. Introduction [CCC11, KKL+12, LP10a, ¨OS10a, ¨OS11, PBL12, Sch12b, SE11, Tch11, BC15, BC16, KCK14, KSAK17]. Intuitive

[OS10b]. Invariance [Laz14, Kon10]. invariants [LZ10]. Inverse

[CCA+12, Kar09, LXD13, WR14b, BMB12, BN11, CYK17, JW18, KM12c, PT13, WR14a, Kar10]. inversion [Dl18, MMM16, NKWT19, PM12, SH18a]. inverted [AAHN16, BW18, KMT+12]. investigated [CP16]. Investigating

[BS14, MB15, CHSO13]. Investigation [EA16, Gan14, HLBI9, HWWW18, KG17, KLK13, KCK14, SM12, VO12, ASMP15, ATM17, AAA12, AZD+11, BXR+13, BAA+18, BWE16, Buc11a, CZJJ12, CHM+17, CNSK11, CC11a, DDGY12, DMG10, DOE+14, DSVP15, Exn11, GWJ12, HDQ+13, WHZW11, HCL13, JFT13, KB13, KSSK16, Kim19, LB14a, LOHB13, LRP+11, LPO+12, LL11, LDW+11, LXD13, LNZ+17, LMCZ11, LCZL11, LW15, MWH15, MCP10, MPTR12, MB14, MHO18, MSK11, MJ14, MMV+19, MLK17, MLB+10, MKW11, NFD+10, OT14, ONK+13, PZ19, JIP10, PMAP12, PSK+13, QSL10, RK14, RFMC19, RW11, RMP+14, Rua10, SAG13,
SMRK18, SS18b, SR13, SAHAA16, SDM12, TZ11, THVP14, TD19, WGLX10, WXB+11, XZL+12, XCY15, XZG+18, XF19, YLH+19, YJ17, YLW+13, ZHI2, ZR13, ZSHL14, ZZC15, Zha17, ZQW+17, ZL12, ZYL+13, ZMZ13, ZCG+16, ZMB+17, dCSDdmMC13, dSdSPG11, dSTH17, GFRdG11, XWC10.

Investigations [Bou12a, BL12, Cas15, DSSM19, Kim13, KRG+13, Mag14, MSNP18, NMMP14, SSS+10, SLZ+11b, SLZ+11c, SLZ+11a, SLS+11, SM14c, SM14d, VSN+11, WFS13, YL11, ZZR+12, ZFS+11]. involve [Bud12].

involved [CLXZ12, MM10]. Involvement [LSL+08]. involves [ZZ18].


iodo [LZD+11]. iodo-perfluorobenzene [LZD+11]. ion [ABS13, AB16a, Ali19a, BS14, CDS+18, COP16, DLO16, DCHC11, EHKD11, EKD12, FBRBR12, FDMR11, GFB12b, GH11, HMI+15, HJLZ11, HFL+17, IAA15, KMS+11, KME+18, KLK13, Kim18, KUS19, KHH10, LJK+18, MS14a, MHZ18, MPT12, MHOG18, MNC12, Ng12, Oni10, Oni12, SSP+17a, SSZ+10, SLZ+11a, SLS+11, SLZHI2, Vik13, WFS13, XLAG12, YW11a, dSSF16b, dSSF16a, SSP14]. ion-covalent [ABS13, AB16a]. ion-neutral [FBRBR12]. ion-pair [SSP+17a]. ion-stabilized [KUS19]. Ionic [BBW10, AFC+10, AVG19b, AVG19a, Ber13c, Bucl2a, DLZ11, HFL+17, KME+18, MFK+12, MHOG18, NDH10, RI19, RF10, WZZL10, XW10, ZP15, dOLdV13]. Ionization [MAPS18, VAT12, AGB12, CHH+19, DLD15, DVP18, FMCA11, GZMC11, HMM+13, Kit17, LDKB15, PUH+11, PM16, SVPTM+10, SOM10, TGRP19, VF13a, YÇÖ11]. ionized [Glu13].

ionochromic [FBU+11]. ions [ASHF13, BMTT11, BSPK11, CCM08, DSC+11, DP16, FBRBR12, KWL515, KWWH18, KLK13, KFY+12, LLZ10, MKG+11, NC11, RP16, SB16, SKL10, WLG+11, WHM14, YYI+12, ZCG10].

IPR [KK12a]. IQA [JNY17, MC17]. IQF [MC17]. Ir [ZQW13, BBB+12b, BWB+18, CF111, DSD18, HMM+13, KBMM10, MSK11, ÖEDB11, RDB18, RDB19, VF111, ZQJ10, SHW+13, TGA+11].


isomerism-induced [MMSC19]. Isomerization [CFC11, LVP12b, CWSZ13, GK12, GLOGM+11, MB13, NTGC19, PL18b, SSdS17, Tap15, VF13b, WCS+13, TTD13]. Isomers [OPP+14, CW16,


L [CCL\textsuperscript{+10}, DPDR11, MLW10, ZQJW13, WHM14, KSG\textsuperscript{+12}, PUH\textsuperscript{+11}, QTCL10, ZYL\textsuperscript{+13}]. \textit{L-} [PUH\textsuperscript{+11}, QTCL10]. \textit{L-ascorbic} [ZYL\textsuperscript{+13}]. l-cysteinate [WHM14]. \textbf{L99A} [DFF\textsuperscript{+13}, L99A/M102Q [DFF\textsuperscript{+13}, LaAlO [Oni10]. labile [YIY\textsuperscript{+13}]. laboratory [IM15]. laboratory- [IM15]. ladder [CEM14, Jan13]. ladder-like [CEM14]. Ladik [XTLA14]. LaF [Lan10]. Lagrange [Mit11c, KRC\textsuperscript{+16}, OPC17, WWL17]. Lagrange-mesh [OPC17]. Lagrange-sinc [KRC\textsuperscript{+16}]. Lagrange-type [Mit11c]. Laguerre [SMOD11]. Lamb [Rit12a, Rit12b]. Lamé [MFLK10]. landscape [DVC14, PP14]. landscapes [AG10b]. language [Tch16]. LaNiInH [OA12]. Lanthanide [XYL\textsuperscript{+18}, FS11, OAC17, SSW16, TG13, VBJK18, WLG\textsuperscript{+11}]. Laplacian [CWW12, LGL\textsuperscript{+19}, LZZ19]. Laplacian-based [CWW12]. Laplacians [LWY19]. Large [DFF\textsuperscript{+13}, SN15, BHMN19, BBB\textsuperscript{+12a}, BBB16, CKYR18, DFV\textsuperscript{+12}, GFRdG11, HSS18, KP11, KYH\textsuperscript{+13b}, LSKM19, MSS11, Mit11c, OCL\textsuperscript{+18}, PBB15, QSX\textsuperscript{+15}, RAMB18, TY17, Tok16, UDS19b, XXJ\textsuperscript{+16}, YFY17, ZWSF16]. large-amplitude [XXJ\textsuperscript{+16}]. Large-scale [DFF\textsuperscript{+13}, SN15, CKYR18, RAMB18]. larger [JLL\textsuperscript{+18}, MSNP18, RVNP12]. Laser [BN11, RP11b, DLCB15, GV19, GRLA18, HYH\textsuperscript{+10}, IAA15, NWQX11, SRPD16, SVPTM\textsuperscript{+10}]. later [Mur12]. lateral [LEU\textsuperscript{+11}, SIT\textsuperscript{+12}]. Latin [CJBMMAPR19, GRCGRRT19, MCCGM\textsuperscript{+19}, MNCNV19, RA10b]. lattice [DTFK15, Ng12, PK13b, VBC\textsuperscript{+12b}]. lattices [DB13b, VBC\textsuperscript{+12a}]. law [BR10, BR16]. layer [Kim18, RTG\textsuperscript{+19}]. layer-structured [Kim18]. layers [ATS15, Dw13]. laying [KHH10]. LCAO [Nal13]. Lck [XFW14\textsuperscript{+12}]. LDA [Fuk12]. Lead [VDG13, CAA19, MW15, Per10b, VVY18]. Leading [LG12, KMS\textsuperscript{+11}, YY18a]. Leading-order [LG12]. learned [LSP\textsuperscript{+16}]. learning [BR15, CLKD15, FLvLA15, MJSC18, NDLC19, Rup15a, Rup15b, SKLC19, STM17, vLRRK15]. Lee [LJ16]. Legendre [Win10]. Leibler [LSS19, LNV\textsuperscript{+18}]. length [Mar11, PE11, RKCK19, Sch10b]. Lennard [CAP12]. lesion [SM13]. lessons [PR10b]. Letter [HS15, PS14, Sha11a, dFR15a]. Letters [CK13, COP16, Lad14, Lun13a, Man16, MBSAG16b, PS13b, Tou13, VV13, VUC13, XTLA14, dSSF16a]. level [AOT\textsuperscript{+18}, AST19, BldV19, KK13, KdSM\textsuperscript{+10}, LCL\textsuperscript{+10a}, MAN15, NBI\textsuperscript{+10}, PAD\textsuperscript{+10}, PWH\textsuperscript{+12}, RNE10, Shi13, SZL\textsuperscript{+14}, WWHZ13]. levels
[OD12]. MD [AHC+18, Eil14, MFB11, SLA12, YWY+12]. MD/ QC [Eil14].
MD/QC-simulated [Eil14]. MD/QM [MFB11]. Me
[CFC11, GWM11, HHL14, RBTL19, HHL12a]. mean [DCD11]. mean-field
[AGNS14, BL10, Nèm14, OK16, RNdA+10, TH12, ZXY13]. measurement
[Eff10]. measurements [Bra19, KDA+11, ZPM10]. measures
[Ale13, DTPC17, I0018, Kan18, LS17, LS19, Lat13, LRMA19, Luz13,
MR18b, SLG11, YOS15, ZYL+14]. MeB [CFC11]. mechanical
[CPAT11, DKR10, DC14b, LV19, MMP+18b, MPD+10, MPL+11, Pan19,
PP19a, RDM+11, SSA18, VPF10, XS18, YZ12]. mechanics
[BBB+12b, EAH13, IAK13, Ma14, MPE15, MSC10, Rup15a, Rup15b, SK17b,
SIB+13, UV18b, Brä12]. mechanics/molecular [Ma14]. Mechanism
[KBF+13, MCC13b, Pl18, SH18b, WML10, ZQW+17, ZL10, AG10a, Bal16,
BCP10, BL11, BLWJ17, yBZ18b, CCL+10, CWS15, DS12, DP12, DZ11a,
DSZB18, EAH13, EM17, FZX18, FMDR11, HWZH11, HhGqZZ17, JSLL14,
LGM+18, LJK+18, LLL16, LZW+18, LLBqD+19, LS19, LWJL10, LMC+10,
LCM+11, LCS+11a, LCH+11, LCS+11b, LXX11, LLLL13, MLW+14,
MOSK10, MR11, MML+11a, MKW11, NE11, OH12, OH13, PL18b, PO15,
RY12, RFMC19, SAS+12, SSI+10, SAG13, SKS10, SKS11, SDR+13, SDM12,
SR18, SLS+15, SZL+15, SSD17, TM13, TLY10, TXL10, VPG12, VML+11,
VOK+18, WGLX10, WXZ+11, WHS+13, WWLZ17, WWX+11, WLD+10,
XDM+10, XZCH11, YM12, YNL18, YWJ+11, YZHZ15, ZRGE+19, Zha10,
ZZW11, ZCZ+12, ZBK15, ZBG+19, ZSS+13, ZCTG18, ZTC11, ZLY+14,
ZPW16]. Mechanisms [CGIA12, LLF17, LFTL18, PWL+10, XZG+18,
AGN14, CWZ+10, FTB11, HLJZ11, HZX+19, HNSB18, HYZ13, JLS13,
LNGW14, LD17, MXC18, MMP+18b, MLB+12, NKWT19, NZLG15, OD12,
PTS+11, PRG+10, RFGGFP+16, SYK+12, SSK+12, SS18a, VHTG15,
WLWT12, YSS+10, ZPB12, ZMZ13, ZSHL16]. Mechanistic
[Buc12b, GMT18, LTL18, LKZ+16, NP18, SGL19, WWR+18, dSM19a,
AASU+17, AEAS+19, RNdA+10, VPO19, dLIAI+12]. mechanochemical
[TJS17]. mechanochemistry [QBRA18]. media [CPL15, Ser11a].
mediated [Dau16, FMDR11, SGL19, WTP+19, ZL10]. mediating
[Var14, ZYL+14]. Medium [TBRIS12, BRIS10, BB16, EAK+10b, EAK+10a,
MPCM+11, PBB15, Puz16, Ser11b, TV13, TBRIS10, TBRIS11, XDM+10].
medium-sized [Puz16]. medium-to-large [BBB16, PBB15]. MEDIT
[ZRGE+19]. meeting [Tch13]. Meetings [AIGZ12]. meets [Puz17].
melamine [AASU+17]. member [RVN+12]. membered
[ABTW14, BBKO16, MSK11, VwRSW+11, Zha14]. membrane
[FMP+17, KMT+12, SMK+12, YINM13, MMP11]. memory [BXR+13].
mesityl \[KDC\] . Meso-\[IMS+13, MMF+13, NKF+13, OH13, She13, YMY+13, VSN+11\]. Meso-substituted \[VSN+11\]. mesogen \[RS11b\]. mesoscopic \[Lun13a, Lun13b, Tou13\]. Metal \[KSG+12\]. Meta-GGA \[KSG+12\]. metabolism \[DKZ+10\]. metabolism-based \[DKZ+10\]. metabolites \[LCG12\]. metabotropic \[´SKB18\]. metadynamics \[BVRM10, MBS+18\]. Metal \[RdPW+12, ZFC+17, ASHF13, ADR+18, BWW10, BHMN19, BEM11, BZBZ13, BDG17, BLdV19, BB10, BDR12, CPF12, CW+16, CP13, CFČ11, DS11, DDS18, DMBJ15, DD17, DP16, ENV15, Esr18, ESLM19, FM16, GM11, GZBH18, HSN+11, Hog13, HWWW18, JHL+18, KWC11, KFY+12, KT12b, Kry12c, L12, LYW+19, LKD+16, MHZ18, MLW10, MC17, MPT12, MVG18, MBA+19, MLW16, NKWT19, NZ13, NFD+10, OKK10, PSK+16, RCM+19, RC13, SFL+10, Sat11a, SG19, SHE10, SK11, SM14c, TTD13, VSMK13, WCY+10, WLL19, WR15, XS18, XG18a, YLW+13, YLZ+17, ZK12, ZLW16, ZHI17, ZSZ14, HZZW11\]. metal-flavonoid \[DS18\]. metal-free \[BDG17, ENV15, Esr18, FM16\]. metal-insulator \[BEM11\]. metal-ligand \[CPF12\]. metal-organic \[MLW16\]. metal-pentagon \[LYW+19\]. metal-sulfur \[LKD+16\]. metal-to-ligand \[DS11\]. metalted \[MSOV13\]. metallaboranes \[SALK19\]. metallic \[AM10, CRB+12, Nic11, VG13\]. metallicity \[AAAM12, AAA12, Kan18\]. metallocene \[OD16\]. metallocyclophanes \[BH10b\]. metalloenzyme \[dCDC+11\]. metalloenzymes \[SSI+10, SS+12, SIS08, YSS+10\]. metallocrofere \[HLB19, SUL+11\]. metallofullerenes \[LYW+19, WLZ+12a, WSL+11, YL11\]. metallophilic \[LC16\]. metallophthalocyanines \[ZDZO10\]. metalloporphyrins \[CCL+13\] . metals \[BMRM19, DW+16, HNBS18, JEA13, JL12a, MK11, Pie11, SAHG11, TMC+13, XYL+18, ZFC+17\]. metals-encapsulated \[JL12a\]. metastable \[DSSM19, MTS15\]. metastable-bound \[DSSM19\]. methacrylate \[DSRG12, IBA+11\]. methamidophos \[SZL15\]. methanation \[LZW+18\]. methane \[AG19, BPSM12, CAP12, SSI+10, YRN+11, ZAK13\]. methanogenic \[SL+10\]. Methanol \[VLK+11, XGH+18b, BCF+11, GB18, KBF+13, LGM+18, LCB10, RYM12, RYN+12, SCBP17, ZSHL16\]. methionine \[TBHL11\]. method \[AAHN16, AHT12, Anc+15, BDF+16, BW15, Boe12, Bu12a, Cam10, C10, C10L, CR18, CFOC+10, CNSK11, CCI9, CYK17, CC12, CF14, DK13, DW12, D13, DCR10, DLS18, D16, FYhC11, FKL+12, FZC14, FRC10, FNT16, GR11, HKZZ15, HSN18, Hor13, HZS14, HM10b, HM11, HBM11, IFT13, IFT14, ISN13, IN15, JH15, KRC+16, Kar12b, KSS12, KL13, KCK14, KHY+13b, Kit15, KFY+18, LdMCdA+12, MM19, MMG15, MdAdCS12, M16, MR11, MAF19, Mit11a, BBSMJC18, MA10, MB12, NZ13, NL11, Osi11a, Pul11, SM11, SY10, SA11a, SS12a, SN15, SGH10, SLZ+11a, SM11, Szi18, TKN13, VAT12, Viv19, WWL17, XLGA12, Xu16,
methodologies [RSCS10]. methodology [CF11, FCC11]. methods [Brä13, Hor13, IFT13, MSH13, Mar13, YK13, ZJS13, dGR14, AF19a, BLRdA+10, CP10, CCC19, CC19, CKB18, DGA+13, DFV+12, Exn11, Gag11, HCH+18, HNH+12, Hat13, HJK14, HJ13, JW18, KKH18, Kon10, LP10b, Lya14, MPM15, MC17, Mar12, MBA+13, Mit11c, MMP11, NC11, NDP10, NMSR14, Nym14, PDR+14, PI13, Pie11, dSMPRSF18, RFEGPP+16, RS11b, RSCS10, SGB11, SOF+10, Sch12a, Sza13, SPM+15, Tok16, TG13, UYN+13, Var11, WKE17, WH12, WCM14, WZX15b, YZ13, YKM+15, YWY+12, ZDO10, ZXY13, ZKW17, dHLdS12].

methyl [SC12a, SC12b, CMCN11, DDC¸Y12, DP12, FO10, HYZ13, IBA+11, IK14, KC11, KSAK17, LD17, LSG+14, MFR10, NAK+17, NZAVR10, Owe17, ÖEDB11, PGG12, PCR+11, SLS+10, SHW+13, WZZL10, Zha14, KAOB11].
methyl-5-methoxyphenol [KAOB11]. methyl-substituted [NZAVR10].
methylene-3-methoxy-cyclohexa-2 [KAOB11]. methylation [BS14, CAAI12, JS18, WYWL13, YPDW14].
methylation [BS14, CAAI12, JS18, WYWL13, YPDW14].
methylation [BS14, CAAI12, JS18, WYWL13, YPDW14].

methylation [BS14, CAAI12, JS18, WYWL13, YPDW14].

methylation [BS14, CAAI12, JS18, WYWL13, YPDW14].

methylphosphonate [HYZ13]. methylsubstituted [KBMM10].
methylbutenol [AEAS+19].
methylcyclobutyl [KDC¸12].
methylcyclohexylidene [KGVG11].
methylcyclohexylidene [KGVG11].
methylcyclohexylidene [KGVG11].
methylcyclohexylidene [KGVG11].
methylcyclohexylidene [KGVG11].
methylcyclohexylidene [KGVG11].
methylcyclohexylidene [KGVG11].
methylcyclohexylidene [KGVG11].
misuses [PIS18]. mixed

[CP11, DKS11, FDNR10, HFBC19, KL11, KSY+11, Lad14, LJW+11, ST15, SN12, TPCj+12, XTLA13, XTLA14, YIY+13, YSK+12]. mixed-quantum

[CP11]. mixed-quantum/classical [CP11]. mixed-valence

[FDNR10, KSY+11, TPCj+12, YIY+13, YSK+12]. mixtures [HFL+17]. Mk

[NYS+10, SKHN13]. MK-4965 [SKHN13]. MLi [SM17]. M’M

[MLY+16, AHC+18, AHC+18, AMMK11, Cap16, DGM10, Exn11, GFRdG11, MOLF11, MG10, RNC+14, SDP+16, SD16a, SD16b, ST15, SLA12, UYN+13, VHTEG15, ZKW17, dAGNJT12]. MM-ER

[TIKN11]. MM/continuum [Cap16]. MMPs [TPdMB12]. MN

[PAKA15, BXR+13, BDR12, YL11, KLk13, Kim19, MRT11, NKWT19, PM17, SAHA12, TMM+14, YYY+12]. Mn-superoxide

[PM17]. MnXMn

[YIY+13]. MO

[ZLY+14, HNBS18, MLY+16, MGP16, PP19a, BB10, Bou12b, Nal13, DWPK14, GD11]. MoB

[BG11c]. mobile [SL13]. mobilities [UDS19b]. Möbius

[GXZ+14, LGL+19, WWL+11]. Mode

[DJ95, DJ12, LYD+18, PVS12, SSI+10, ST15, SD12]. Model

[LEU+11, ASD18, AMAM18, BPL13, BEM11, BGF14, BAA+18, Bkm15, BH10a, Buc11a, Buc11b, CPF+11, Cam10, Cam12, Cap16, Car19, COCF+14, CnSK11, Cscvb12, Cys11, Dzo12c, DqF12, FMP+17, Fb17, Fs11, GlogoM+11, Haji18, ISM+13, JK12, JzP17, KyHi13a, KbJ17, Kkg12, Kb12, Llf+12, Ldkb15, Lsr+13, LkJk13, Liiu15a, LnLi12, Ly19, MyYz+10, MMp+18a, Msh13, Mgg+11, Mrt11, Mpe15, Ma12, Mt10, Mni13, Pabsk16, Pwl+10, Pcr+11, Rtg+19, Sppt15, Smgzf19, Skk11, Spsa11, Sks10, Sl10, Sm10a, SLS+19, Srn+19, Ssd1s17, Tgr1p19, Vie17, Vgs10, Wml11, Wwqg17, Zen11, Zlzj11, Zzz+18, dOr10]. modeled

[Mmbk12]. Modelling

[Brs10, Iba+11, Kry12a, Lbm11, LC19, Men15, Mra11, Nbzt16, dsmprsf18, Pog12, Tbb+19, Tcm+12, ZpZ15, Z19, AHC+18, Bgf14, Buc10, Crsbl2, Cskk+12, Dsm+19b, Dfk16, DLM+11, Ddp+12, Fbo+11, Gma+19, Hl19, Kms+11, Kbj17, Kgg12, Kb12, Llf+12, Ldkb15, Lsr+13, LkJk13, Liiu15a, LnLi12, Ly19, MyYz+10, Mmp+18a, Msh13, Mgg+11, Mrt11, Mpe15, Ma12, Mt10, Mni13, Pabsk16, Pwl+10, Pcr+11, Rtg+19, Sppt15, Smgzf19, Skk11, Spsa11, Sks10, Sl10, Sm10a, SLS+19, Srn+19, Ssd1s17, Tgr1p19, Vie17, Vgs10, Wml11, Wwqg17, Zen11, Zlzj11, Zzz+18, dOr10]. moles

[Bj95, Dj12, Lyd+18, Pvs12, Ssi+10, St15, Sd12]. Models

[Leu+11, Asd18, Amam18, Bpl13, Bem11, Bgf14, Baa+18, Bkm15, Bh10a, Buc11a, Buc11b, Cpf+11, Cam10, Cam12, Cap16, Car19, CoCf+14, CnSk11, Cscvb12, Cys11, Dzo12c, DqF12, Fmp+17, Fb17, Fs11, GloGM+11, Haji18, IsM+13, Jk12, JzP17, KyHi13a, KbJ17, Kkg12, Kb12, Llf+12, Ldkb15, Lsr+13, LkJk13, Liiu15a, LnLi12, Ly19, MyYz+10, Mmp+18a, Msh13, Mgg+11, Mrt11, Mpe15, Ma12, Mt10, Mni13, Pabsk16, Pwl+10, Pcr+11, Rtg+19, Sppt15, Smgzf19, Skk11, Spsa11, Sks10, Sl10, Sm10a, Sls+19, Srn+19, Ssd1s17, Tgr1p19, Vie17, Vgs10, Wml11, Wwqg17, Zen11, Zlzj11, Zzz+18, DoR10]. modeled

[Mmbk12]. Modeling

[Brs10, Iba+11, Kry12a, Lbm11, LC19, Men15, Mra11, Nbzt16, dsmprsf18, Pog12, Tbb+19, Tcm+12, ZpZ15, Z19, AHC+18, Bgf14, Buc10, Crsbl2, Cskk+12, Dsm+19b, Dfk16, DLM+11, Ddp+12, Fbo+11, Gma+19, Hl19, Kms+11, Kbj17, Kgg13, Ltsdj+10, Lzz12, Mali4, Mpj12, Mcv11, Ovt+16, Ptd+12, PIS18, Rdb19, Rbtl+19, SjzL12, Sic16, Sls+10, Sr18, SkbJ18, Sm14a, Ssb+12b, Tay11, Ybmk12, YJ17, Zp16, Zk12, dagnjt12, dssdsaga12, Kmg13]. Models

[FFF10, Am13a, Adr+18, As19, Ali19a, Bmr+13, Bm16, Buc12b, Cww12, Cpat11, Cst16, Eps+16, FlvlA15, Gmt16, Hvr18, Jcc10, Ko10, Lvdsd14, Li15, Lorr+12, Lskm19, Lwh+12, Lz10, Luz13, Mpv+11, Ns10b, OpaV18, Pii13, Pl11, Qbra18, Rfeggp+16, Sktt15, Sjw13, Tdi11, Vlg12, Wym15, Wh18, Yyi+12, vlrRk15]. modern

[Hat13, Ly19, Tbb+19]. modes

[CLXZ12, Fkc12, Hax+18, Pm12, RpBB11, RAl0a, Tu10]. modification

[KK19, Wan11]. modified

[DJ18, HfZ12, Lzw+15, Psgk17]. modulated

[HGB08]. Modulation

[Msi14a, Gv19]. MODYLAS

[YAF+15]. Moeller

[EG10]. MOFs

[Pk16]. moieties

[Cha11, NCMC+18]. moieity

[BS14, ElC08, Skm11]. Moisseyev

[Brä12]. Molecular

[Buc11b, Css16, Cskk+12, Chv14, Dgr+16, Dlz11, Fkb19, Fue+12,
Hor13, IHG10, KTI+12, KM12c, KKT13, MY17, MAD12, MSH13, Mar13, MP12, MOY13, McCi3a, MMT+13, MBS+18, NVI10, OHDA13, OA13, Pvs10, PWH+12, PPK+13, RAK10, SMK+12, SIT+12, SVPTM+10, SIB+13, SHS+13, TpdMB12, UYN+13, UTN13, VHTEG15, WML11, WWB+14, YK13, YINM13, dSSdSGA12, AC19, AV19, AS19, ABA11, AA15, Bae14, BL16, BBB+12a, BPT12, BDF+16, BMF+14, yBZfC18, BMB10, BBB+12b, BR15, BWB+18, BWE16, BH19, CRA+11, CDK12, Cam10, CZJZ12, CTVA12, CVC+16, CFV18, CD15, CNSK11, CHL+19, CAPL12, COP16, Dau16, DSD18, DDC¸Y12, DI18, DLM12, DDG+11, DDVX12, Eil14, ESLM19, FZH+18, FBRBR12, FMPP+14, For12, Fra17, FBU+11, FSST16, Fuk12, FDG18.

molecular [GVPCK10, GFB12b, GI11d, GH11, GJ18, GSPR19, GR10, GHP11, GS10, HS11a, HYZ12, HYZ19, HLB19, HII13, Hog10, HZS14, HFL+17, HVR18, HFBC19, IFIT13, IA13, IKC18, Ish14, JdL08, Jan10, KLM13, KCK14, KHH10, KKH+13, KKT14, Kry12a, KRG+13, KU16, LB14a, LG10, Lai11, Laz14, LML13, LA11, LTdSJ+10, LFS+11, LJS12, LG15, LC19, LKLW11, LNI12, LB18, Ma14, Mam14, MC11b, MHT+08, Mas14, MOE+11, MMBK12, MKG13, MAF19, Mit11a, MSY+12, MSK+12, MVA19, MPL+11, MLB+10, MIBTR12, MBBT+12, MBA19, MMP11, Mri12, NKK15, NDH10, NAK+17, Nic11, Nik11, NB19, OT14, OB19, OWD18, PP10, PMH+16, PH12, PBB15, POG12, PET18, PRG+10, Puz16, RS12b, RSM12, RBGGM18, RAN18, RMC19, RP16, RL14, Rit11, RC11, RAMB18, RdPW+12, RA10a].

molecular [SC12b, SLZ+11b, SXS+12, SLS+12, SLSZ13, Shi13, SRS+17, SACA18, SLS+10, SKY+13, SWS12, TK16a, TY17, TFA10, Tok16, TSH17, TIKL13, TRZ+19, TC12, TPT19, Vik13, WZ10a, WFS13, WC14, XFW+14, XXJ+16, Xu16, XWP+18, Xu19, YZH15, YAF+15, YT14, ZSASS13, ZHF+13, ZPR10, ZLE17, ZLW16, ZRLV10, ZB18, dSSF16b, dSSF16a, dOdCMUdALR11, dWLC14, dOLd1V13, vL13, vLRRK15, Puz10, RI19, RdA11].

molecular-dynamics [PP10]. molecular-level [Shi13]. Molecule [ANC+15, AM12, ASK15, Ber13c, CAZ+11, CI11, CHM+14, CHM+17, CC11b, Cor16, DAC11, DAC12, DAR+11, DPRK12, DLG12, DCZ17, ES17, Esr18, Fra17, GWH17, GI11a, GT13, HK11, IIS+17, KKH18, KSC15, KP12, KN15, Lan10, LJS12, LEU+11, Luz11b, MGM11, MHT+08, MSS11, MKD19, MZLM17, MPTZ13, MJM19, MC18b, OT14, OCL+18, PK13a, RPPB11, SXS+12, SLSZ13, SLZH12, SRA+11, TFBG14, TH12, Tob19, VOAH18, Vik11a, Vik11b, WR14a, YW11a, ZZZ+18, KRC+16, TFSRM11].


molecule-to-material [TFBG14]. molecules [Agb12, Ale13, Ali19a, ACL12, AT18, BMK+14, BdTG11, BCHN16, BRS10, BAX+19, BDG17, BOMB16, BB10, Cam12, CM17, CPL15, CRSB12, CKB18, CB19, CK17, CF17, DIOG12, DK13, DSRGD12, DI13, DCR10, EML+11, EMS16, GFB12a, GMR18, Gin10, GS11, GHP11, HRT12, HMH+13, HST13,
molecules [SMEH15, Sha18, SB16, SMR14, SRN19, Sto18, SYY16, Sut12, SCZH16, SV11, THL15, TK16b, TH12, TXK19, TFMC19, Tou11a, UGWL18, VO11, XHZXXZ10, YZZ16, YD17, ZS11, ZDF13, ZP16, ZCC11, ZZZ18, ZS12, ZI19, dSCC12, dSTH17].

Møller [RS11a, BVA14, NMIP14, RS09, TH13]. molten [BM10, DLZ11]. moment [AM10, Ber13a, DPRK12, GFB12b, GI11a, GI11c, LMC19, MD11, TW10].

Momentum [SH19, ALRA10, Ash18, AKR12, HSN18, MOY13, TCG17, TÁ10, YOS15].

Moniliophthora [PTD12]. mono [Buc12b, DHYC19, Jac12, MMR10, PS13a, ZQXP17, BL10].

monoacetylides [DD17].

monoamines [MBTVR12].

monoatomic [Bar11].

monoboronyl [MLK17].

monobromide [HTM10].

Monochloride [MOY13].

monodentate [ZKKR11].

monofunctional [XZ11].

monofurazan [ZZX10].

monohalogenated [MNV17].

monoiode [HTM10].

Monolayer [UDS19b].

monolayers [KC19a, MDP12, RZC13, TTM16].

monolithiated [WWL11].

Monomer [Cas15, BHA19, JWG12, MM13, BMR13].

monomeric [Rua10].

monomers [MBA13, UJSJ13].

Monomolecular [MOKS10].

monooxygenase [SSI10].

monophosphates [PAD10].

monosulfur [WJ11].

monovinyl [dlLIAI12].

monoxide [AKC10, Hog13].

monoxides [TG13].

Monte [AFV12, ABG12, ANC15, ASK15, Cal10, CKB19, CCC19, CP16, HCH18, Hog13, HBU14, HM12, JCCZ12, PDR14, PIS18, RCGLV14, SG13, SCBP17, Wag14, WCM14, ZLR15, ZCC11].

montmorillonite [BJdlMAV12].

MoO [MFZ18].

moracin [MGK12].

mordenite [NL11].

Morita [ZQW17].

morpheine [RCM10].

Morse [Agb12, PSGK17, Sta10, Tou11a, ZLJ11].

MoS [LZW18].

Mostar [ACT19].

motif [SLZ12, YD17].

motifs [CJMC19, KUS19, Kry10].

motion [Cam10, DKR10, KCDC15, KC18, MMCN11, MMSC19, SRPD16, Sut12].

movements [HZW18, XXJ16, YW11a].

motors [OWD18].

moving [FAFR12].

MP2 [KBMM10, LKLW11, NMIP14, yOITn15, RSM12, ZS11, Tav12, Yu13].

MP2-F12 [yOITn15].

MP4 [SZ11].

MPI [CwCW11].

MPI-2 [CwCW11].
MRCC [NYS+10]. MRCI
[DAR+11, LJSS12, Mit11a, ONBP11, SLZ+11b, SLZ+11a]. MRI [GSPR19].
multiconfiguration [Gag11, HJK14, KK14b, Luz13, NS13, PP16, Pie11, SY10, VMR11].
multidimensional [Kha16, SIB+13]. multielectron [Kry11b, Kry12b].
multiexcited [SCZG12]. multimode [RGPZD13]. multiobjective [SSB12a].
multiparameter [GMGRMP12, IIH16]. Multipartitioning [RS09, RS11a].
multiphoton [NWQX11]. Multiple [HhGqZZ17, PBM10, PP14, DB12, GFRdG11, Ish14, JW19, MGB18, NMV+14, RWW+19, YGLL10]. Multiple-pathways [PP14]. Multiplets [BMB16].
multipolar [TH12]. Multireference [CYLL11, KB19, LP10b, RMG+19, SWS12, BPV13, GSAY11, HFD11, JNZ+14, Kon10, MdAdCS12, SYL+18, SLZ+14a, dSM19a].
Multiscale [ACH+18, Mas14, ZP16, CLKD15, CwCW+11, MGN14, TTM16].
Multistep [SAS+12, Sic16]. Multithreaded [MAF19]. multitopic [SSP+17a].
multivacancy [MFM18]. multiwalled [LV19, MNS11].
multiwavelet [HS11a]. munchné [GHCMCMQ17]. muon [RAGM10].
mutations [DMG10, MFR10, MG10]. mutipathways [SWS+14].
Mutual [Mat02, MAT19, Mat10]. Mycobacterium [ST15]. myoglobin [CHSO13].

N [AGOP18, BBYZ18, BJ17, CJMC19, CWS15, CWSZ13, GC18, HWL16, JLG+12, Kal18, LYL+12, Men10, MC18a, OCL+18, PCK19, Per10b, RLTAT19, SB18, SABA+12, SSAM13, WLZ+12a, WLZ+12b, XZZ+10, XJJ+16, XCL+18, Zha10, ZH12, ZQJW13, SC12a, ARG11, BEM11, LL18, LYY19, XYL+18, XWC10, ZCTG18, ABTW14, CJCMA9, CTW12, CDL+19, Esr18, FLCHL10, GMM+18, HZZ+19, HM10a, HXX15, KMK+16, KMM+18, LYL+12, LW15, MNV+17, MBA+13, PRPU+13, PL18b, Puz10, RRB12, SABA+12, SC12a, SSAM13, SXS+12, TM18, Tob19, TPDMB12, WZX11, XMZ+12, XZZ+18, YZL+10, YWJ+11, Zha10, ZH12, ZGSM15, ZCG10]. N- [SC12a].
N-confused [HM10a]. N-coordinating [YZL+10]. N-cyclic [XZG+18].
[BSM +15, ZLS +18]. nitryl [BL11]. NL [YFY17]. NLi [YLWrL12]. NLO
[PCD14]. NLO-X [PCD14]. NMR [AM13a, BMF +14, ÇAS13, CCP18, 
CSP +10, CDT12, DSD18, EKN10, FBD +13, GSPR19, MC18a, OPP +14, 
ÖEDB11, Ped16, RRK16, RR19, SK10, TTM16, TKSK17]. NO
[ESS13, LLC +11, SSAM13, STU19, ÄFV12, BAMA12, GMT18, Les12, 
MCV11, OG19, RNB +10, SK14, SSAM13, VLM +10]. noble
[GI14, JEA13, KDOR17, MB15, PSK +16, SMC18, WLL19, XS18, XGH18a]. nodule
[CMZ10]. NOF [PM16]. nomenclature [Tch16]. Non
[BPL13, Cor16, DKS11, Leh19c, SGL +16, Tob19, YLH +19, Brä12]. non-
autoionizing [Cor16]. Non-Born [BPL13]. non-covalent
[YLH +19]. non-dynamic [Tob19]. Non-Hermitean [Brä12]. 
non-interacting [SGL +16]. non-relativistic [Leh19c]. Nonadditive
[BW18, Cys11, RSN12]. Nonadiabatic [GW18, LKd +16, MNZPT19, 
MKD19, WDR +11, YT14, AC12, HKLW13, IHG10, PM12, SBL11, ZI12]. 
nonadiabatically [Kit14]. nonadiabaticity [GJ18]. 
nonautoionizing [DSSM18]. nonbond [BLWJ17]. nonbonded [ZFS +11]. Nonbonding
[HL19]. Nonclassical [SSB19]. noncollinear [GEL18]. noncompetitive
[AMMB +18]. Noncovalent [BMRM19, Wan11, BDG17, HMA +19, JNY17, 
MIKH19, MNP18, M URL13, Sch15, YF16, YFY17, Zak13]. nonempirically [MIN13]. nonequilibrium
[DKR10, DCZ17, Li15, Mar13, MMP11]. nonframework [SZ11]. 
Nonharmonic [RSM12]. nonheme [ASD14]. Nonhydrodynamic [BM10]. 
nonidentity [Buc11a]. noninertial [NF11]. Noninnocence [Joh17]. 
noninnocent [DG19]. noninteger [CG12, GE12b]. noninteracting
[AST16, BEM12, RS13]. Nonlinear [SRMB15, YK11, Yak10, ABA11, BF11, 
BSM +15, BEZP10, CRA +11, CEV10, CKB18, DSRGD12, DB12, FSQ +11, 
HWL16, HWW18, HSS18, IGMK11, JFDD10, KC11, KPL +17, KL11, 
LKD11, LWZ +15, LYL +12, MMF +13, MB12, NKF +13, PCD14, SKG11, 
SM17, SYQ +10, YLWrL12, YHLC15, ZSQ +10]. nonlocal [FMMD +10]. 
nonlocality [BSS16]. nonmetal [JHL +18, WCY +10]. Nonorthogonal
[CC12, DCZ17]. nonparametric [GTSC +19]. nonpolar
[KKT13, KKT14, SA18]. Nonrelativistic [ADB10, RZ17]. Nonsingular
norbornadiene [TDD13]. Normal
[DJ95, DJ12, HAX +18, Pan16]. Normal-Mode [DJ95, DJ12]. normalized
[FZC14, LGL +19, LWY19, LZZ19]. note [RLER13a]. notions [KK14a]. 
Novel [KAG08, VRO +12, WCY +10, WZM +13, CMR13, DW12, DLM12, 
GJWIZ11, JWCG +12, LZZ +11, LZZ +17, NVPCJ +13, Pop15, PL18b, RDM +11, 
SSTÖ11, TpDM12, UJSJ13, XFW +14, XZ11, YZL +10, YSW11, ZZR +12]. 
novo [SBKJ18]. NQR [EA12]. N — [OK16]. NTA [MC17]. NTChem
[NKK15]. NTO [LZZ +13]. NTPA [MC17]. Nuclear
[GR10, MJ11, RLER14, STU19, BPL13, BJ12, CG12, Cyb11, DVDBM11, 
FKL +12, GJ18, JHSG18, MZB +13, Mam14, MVC13, MNZPT19, NS10b, 
NB17, SPSA11, TMC18, ZPM10, ZP16]. nucleic
nucleobase [KZKW17]. nucleobases [CAO18, Cys11, DSV15, KZA+17, LCH14, TD19, WG18]. nucleophilic [Buc10, Buc11b, HLJZ11, Pli18]. nucleoside [HHYC+18, VFSC17].

on-the-fly [UTTn13]. One
[Ber13a, CG12, Dum12, LCH14, Bud12, CAZ+11, CM15, CLY12, CYK17, FCS13a, FCS13b, GTR11, GI11e, GAMM10, GS10, HZS14, Kri13, LW15, Luz11a, MSC10, MBBT+12, PVS12, RZSZ18, SC12b, SZZ+19, SWS+14, TAY11, VBC+12a, VBC+12b, WWC17, WLZ+12b, YF16, ZZZ+18, TC12].
[LRKM10, YBMK12, AMK10, ABA11, BF11, BSM+15, BSO16, CPL15, CZLD17, DWX+16, FSQ+11, FZX18, FBU+11, GAPK+19b, GDM+10, GKM18, GRCA19, Hat13, HWL16, HWWW18, HSS18, IGKM11, JdOS16, JFDD10, KC11, KPL+17, KL11, KMU+13, LLY+11, LZW+15, LYL+12, MPC10, MNP19, Mas14, MPJ12, MFZ+18, MA11a, MMF+13, NFK+13, NMHPVG12, OGVSG18, RKM12, RRVR19, SBAT16, SSS12, SLS+14, SM17, SYQ+10, WLZ+12a, YK11, YLWR12, YHL15, ZSQ+10].
optics [DSRGD12, LKDC11]. Optimal
[FT15, GSPR19, NV10, NB19, TC17, YWR+18]. optimally [NTGC19, ZZ18]. Optimization [CL08, FCC11, HJ13, KYH+13b, Kub12, Lu15, MHT+08, SGH10, SPM+15, WWL17]. optimization [YIY+13]. optimized [ANC+15, KPH+12, SXH18]. Optoelectronic
[AFA13, JR19, BHAI+18, KA13, MANP17, OAA19]. orbit
[Ash18, Ber13b, BDR12, CYL+18, KV19, LWL+12, MLK17, MC18b, RS12a]. Orbital
[BT15, Kon10, AOT+18, AK17, Ash18, ABA11, Bar11, CPF+11, DVBDM11, Fin17, FA17, FPM+14, FC19, GR10, Hog10, HVR18, IKN13, IK18, JH15, KK14a, KLK13, KCK14, Kit17, KKT13, KKT14, KPH+12, KUY16, LB18, MSNP18, MMM16, MAF19, MFL12, MSY+12, MMA10, Mur12, Nag15, OT14, OAT+13, Pir13, PU14, PNC19, RMC19, SIM14, Tal11, TD11, Tsh15, XHZXXZ10, YPDW14, BT17]. orbital-free
oxides
[IKC18, Kan18, NAK+17, PSK+16, RGST12, RKCK19, VGGPdL19, VKF+19].
oxidized [FTB11, RRB12]. oxidoreductase [SR11a]. oxime
[QCW+12, XZ11, YRN+11]. oximes [ZYSW17]. oxirane [BAX+19]. o xo
[ZSAP11]. oxo-titanium [ZSAP11]. oxoacids [CK17]. oxoanions
[HNBS18]. oxocarbon [JFDD10]. oxodithioesters [GCZ+14]. oxoguanine
[YM12]. Oxygen [GLT13, SDY16, AGOP18, CAZ+11, dDGNB10, JAB12,
KCK14, LSR+13, Mor12, MLW16, PMH+16, dSMRPSF18, SCZG12, SBSD18,
VS19, WWHZ13, YYS15, YS+10, YY+13, YSK+12, YYZ16,
dOdCMUdALR11, OD12, YY+12]. oxygen-evolving [LSR+13].
oxxygen-oxygen [SBSD18]. oxygen/nitrogen [YZZ16].
oxogenated [TYN13]. oxyluciferin [SR11b, dSdS13a].

P [ACMRN10, CdAFS+12, CD12, GWZ+14a, GWJ12, KLZQ15, PP14, SB18,
TW10, VV18, XCL+18, ZCG+17, ZPB12, AGOP18, ED16, OD12, RPBB11,
[AB16b]. p300 [DPRK12]. P450 [SIS+08]. P6 [UV18a, UV18b]. Pa
[OM13b]. package [CcCW+11, NKKN15]. packet [Bae16, Cho19, GKT+12,
HDOS12, NTGC19, RW11, SSAM13, YLYC18, ZCG+17]. packets
[OHDA13]. packing [PETB18]. Padé [DB13a, ZE18]. PAH [CM17]. Pair
[TH13, BKM15, CCL+16, CFV18, HMM10b, LJK+18, LRMAA19, MT11,
NMS+10, OM13b, RS12b, RS11b, SSP+17a, SLG11, TRZ+19, Var11, WH12,
ZBK15]. paired [RLZ12]. pairing
[ACF+11, EMS16, PS10a, SM13, VBC+12a, VBC+12b, ZKWZ17]. pairs
[BTH18, BMB16, HL19, KME+18, KUS19, Lad14, SMR14, SLF12,
XTLA13, XTLA14]. pairwise [Dob14, KKL+16, PSC15]. palladium
[KSG+12, LSCMSFC19, LW15, PW10, SY16]. palladium-catalyzed
[LW15]. PAN [ZL10, VUC13]. pancreatic [PCML08]. Pandora [TFBG14].
para-hydrogen [NG11]. paradigm [SLS+19]. parallel
[CLKD15, Iya19, yOITn15, PCV19, SPBD16]. Parallelization
[ZWSF16, MAF19]. parallelized [SPSA11, YAF+15]. parameter
[FCS13a, FCS13b, IKN13, SZZ+19, SX15, WFS13, YF16]. parameter-free
[SX15]. parameterization [HSS+11, PABSK16, PSPP11, SOF+10]. parameters
[AGPDZ13, AK11, BMF+14, EKN10, FV11, FCC11, GRPR19,
IIS+17, KAR12a, LJJS12, MGM11, MPM15, MOY13, Roy16, SPO+11,
SR11b, SWS12, WDJ+17, YSÖ12, dCSDdMC13, dOdCMUdALR11].
Parametric [BH19, LdMCDa+12, RSCS10, SOF+10]. parametrizations
Part
[Ban12, GI11b, Jör18, Mor13, BR08, BR12a, For12, GI11c, RB08, RB11a].
Partial [MCKD11]. partially [AA11]. Participants
[Ano12r, Ano10a, Ano10b, Ano10c, Ano10d, Ano11d, Ano11e]. particle
DPK18, GE12a, JNY17, JMX+15, Jia15, KJ16a, KJ16b, LSCMSFC19, NKWT19, Obs11a, Per18, PP14, Pul11, Tap15, TBB+19, XXJ+16, ZSZ14.

**Perspectives** [Blo15, BT15, Dob14, HJK14, IAK13, Jan13, JNZ+14, KO14, Kaw15, KJ16b, KJ14, Liu14, LG15, Mak15, MGN14, May14, Men15, MSM16, Nal15, Ném14, NTCK13, Nc14, PK16, RP16, RNC+14, Rus14, SN15, SX15, Sza13, TFBG14, Tok16, Wag14, WYM15, ZLR15, ZLWY13, Zil14].

**perturbation** [BDPT12, CEFMK12, DK13, DB11, DB13a, DCHC11, JHSG18, JNZ+14, Kry12a, LCL+10b, LPG+12, Lin14, NS13, PBB15, RMG+19, RS09, RS11a, Var11].

**perturbations** [DB12].

**perturbative** [PCV19].

**Perturbed** [NH18, Cal10, PVS12].

**perylene** [Cas15, HSS18, JR19, MANP17, WKE17].

**perylene-based** [MANP17, WKE17].

**PES** [QB15].

**pesticide** [HYZ13].

**PH** [AM18, EMSB15, MZLM17, DPDR11, GWM11, Pan16, XCL+18, MPJ12, OAC17, OG19, PJP10, SSP14].

**pH-rate** [SSP14].

**pH-responsive** [OAC17].

**pH-sensitive** [NH18, Cal10, PVS12].

**Phase** [MS12, Nal15, RF10, AEAS+19, BGBV12, Boe12, BCNR18, BLM+12, CF17, DMAB12, DD17, DZ11a, DMB16, DCC+19, EHDK11, FBRBR12, FMKJ14, FDMR11, GV19, GCK+17, GMT18, HCC+11, HDQ+13, HK12, Jen13, JWJ+12, KS11, Kim19, KZZ13b, LKOS17, LNGW14, LGZC15, LGW11, LD12, M11a, Mak15, MCC12, MOSK10, MML+11a, MLB+12, MM+12, NKWT9, NZLG15, Per18, PB10, RP16, RCM10, Riv11, RNE10, SDS19, Ser11a, Ser11b, SK12a, SSdS17, TWR15, VF13a, VV18, VV+16, WXZ+11, WZX11, WL+11, WWLZ17, YC13, ZL10, MJ11].

**phase-space** [HN12].

**Phase/current** [Nal15].

**phases** [DM12, KMU+13, MB14, Sjö15, TFB11, dSDPG11].

**PhCOCOCH** [SKS10].

**phenalenyl** [NKF+13].

**phenalenyl-based** [NKF+13].

**phenanthidine** [BZBZ13].

**phenanthrolinone** [YZW+15a].

**phenol** [CoD+11, HZW18, YY18a].

**phenolate** [ZSQ+10].

**phenolate-pyridyl** [ZSQ+10].

**phenols** [WGLX10, dSNBG08].

**phenomena** [EMED+12, TMC18, ZB18].

**phenomenon** [Bon17, LBdV16].

**phenoxy** [BAMA12].

**Phenyl** [IK14, Bon17, DDČY12, DPRK12, HZW18, LD17, LVP12b, MXC18, SC12a, SC12b, SHW+13, TAY11, TT10, WYW+11].

**phenyl-3** [TT10].

**phenyl-based** [MXC18].

**phenyl-methyl-benzimidazolyl** [SHW+13].

**phenylalanine** [TBHL11].

**phenylaminino** [KAOB11].

**phenylazoaniline** [NVPCJ+13].

**phenylene** [LGL+19].

**phenylenes** [LWW19, MMF+13].

**phenylethyl** [MOH+12].

**phenylmimino** [KAOB11].

**phenylphenol** [NVPCJ+13].

**phenylalkyl** [DFK16].

**phloroglucinol** [MK10b].

**phonon** [DLM12, Lar10].

**phosphate** [Oge17, Pat15, RNdA+10, Rud12].

**phosphatidylcholine** [MKSG13, TTM16].

**phosphazene** [KFS13].

**phosphide** [Kar12b, MM11].

**phosphine** [GWM11, JLZ+17, LFTL18, XZG+18].

**phosphine-boranes** [GWM11].

**phosphine-catalyzed** [LFTL18, XZG+18].

**phosphines** [SAG13].

**phosphinidene** [AKC10].

**phosphinoalkylidene** [XCD18].

**phosphinyl** [Wit18].

**phospholipid** [MP12, MDP12].

**phosphonate** [Oge17].
Positive [FBRBR12, MMRRA10]. positron

[MAT19, SY10]. Possible [KKT13, KKT14, OT14, SSA18]. positronic

[GS11, NGS11, ZS11]. potassium

[MGB18, Sat11a, DMBL16, EM19, ZC1+16]. Possible [MMF18, POLV12, SYK+12, BMF13, KKC14, Kar15, LDZG16]. Post


 Possible [MFM18, POLV12, SYK+12, BMF13, KKC14, Kar15, LDZG16]. Post


 positively [MGB18, Sat11a, DMBL16, EM19, ZC1+16]. Possible [MMF18, POLV12, SYK+12, BMF13, KKC14, Kar15, LDZG16]. Post


 Possibly [MFM18, POLV12, SYK+12, BMF13, KKC14, Kar15, LDZG16]. Post


Possibility [MGB18, Sat11a, DMBL16, EM19, ZC1+16]. Possible [MMF18, POLV12, SYK+12, BMF13, KKC14, Kar15, LDZG16]. Post


Possibility [MGB18, Sat11a, DMBL16, EM19, ZC1+16]. Possible [MMF18, POLV12, SYK+12, BMF13, KKC14, Kar15, LDZG16]. Post


Potentially [CWL+13, FDG18]. potentials [AGJ12, BW18, BC15, BC16, Beh15, BBA+16, Cal10, EI11, ESS13, GMGRMP12, GH11, JH13, KH12, KWW18, Kry12a, KGGK13, LP10b, LH15, MIMM16, MZST16, MBP11, PDR+14, PMGRMP12, PMGMR15, PM16, Roy13, SZZ+19, TH12, Tug13, VLG12]. power [LSC+18, CKB+19].


Prediction [DFV+12, LC12, SGB11, SSP14, Ali19b, BBB16, BBA+16, CPL15, DGA+13, GB18, LCL+10b, LPG+12, PCD14, PWY+18, RMLPGGH16, SLC+18, SRASZ16, SBKJ18, VPD10, VRO+12, WZX15b, YXL+18, YC13, ZYSW17, ZW15, dOLdlV13, MGD11]. predictions [Bou11, Bou12a, KKH18, TSK17, WLL19]. Preface [ACL10, ABC12, Ano13-49, BSS14, DC10, DBMPB11, HSLD14, HB18, NAY+13, NT15, Rei15, RSV10, Rup15a, RA10b], preference [EAH13, JN13]. preferences [KM12b, LB18, MAW+18, NRS+11, NJA+12], preliminary [CC12]. Prelude [AS19], preparation [CS18], presence [DPK18, DB15, EBR11, FRNM12, KSC15, LC14, LB14b, Pit12]. Present [TSvL+16]. Presentation [EMK14], pressure [KMU+13, Mil12, SIT+12]. prevention [Ball16]. primary [ABK18, MOK10, NGS11]. principle
properties

properties/activities

properties

proteins

proton-coupled

proton-electron

proton-molecule

proton-transfer

protonated
QR-SCMEH-MO [BB10]. **QSAR** [KKM+12, MPMCM+11, PH12, XFW+14, ZFW+13]. **QSPR** [CD18, MPMCM+11, SN12, TFA10]. **QSPR/QSAR** [MPMCM+11]. **QSTR** [PI13]. **QTAIM** [BTH18, DP16, MAW+18, NH18, Sha11a, VHTEG15, XXJ+16, XWP+18, YXM+18, ZLZ+14]. **quadratic** [FYhC11, OPAVM18, RSN12]. **quadratically** [ISRK12]. **quadratric** [ZST+10]. **quadricyclane** [TTD13]. **quadrilateral** [LZZ19]. **quadruple** [MPT11, NZ13]. **Quadrupole** [MdAdCS12, AC11, BJ12]. **quality** [OKR12]. **Quantal** [SIB+13, SHKS15]. **Quantification** [SP19, Gru17, ORJ18, Rus14]. **Quantifying** [Mar12, MML11b]. **Quantitative** [CJSNLM11, HSN+11, Zha17, MBTVR12]. **quantities** [FSST16]. **quantization** [HKLW13, Kle11, SD13b]. **quantized** [Tou11b]. **quantum** [ANC+15, ASK15, BF11, Ban12, BAX+19, Blo15, BGL+16, BHH+13, BT15, BT17, BM16, BBB+12b, Bra10, Brä12, Buc12a, BN11, CD18, CKB+19, CM16, CS12, CSG14, CW13b, Cho15, CYK17, Coo12, CPAT11, CN12, Dau16, DPK18, DSL15, DPRK12, Di13, DBML16, DSFT17, EAH13, FLCHL10, FBO+11, FNIT16, FSST16, Gag11, Gan14, GWZ+14a, GRCGRRT19, GB10, GS11, GR10, HR13, HS11a, HITU16, HS11c, HEVMSA+19, HM12, Hor13, HMA+18, IFT14, Ish14, JN13, JHSG18, JMX+15, Kap12, KB12, KCDC15, KC18, Kar09, Kar10, Kha16, KCC13, Kit14, Kit15, Kle11, KN15, KK11d, LS17, LSS19, LV19, LSR+13, LCZL15, LHX+19, Lin14, Liu15b, Liu16, LSKM19, LEU+11, Luz11a, Ma14, MC11a, MR12, Mam14, MDC15, MPE15, Mar13, MSC10, MML+16, MPD+10, MQG13, MPL+11, MBBT+12]. **quantum** [ANC+15, ASK15, BF11, Ban12, BAX+19, Blo15, BGL+16, BHH+13, BT15, BT17, BM16, BBB+12b, Bra10, Brä12, Buc12a, BN11, CD18, CKB+19, CM16, CS12, CSG14, CW13b, Cho15, CYK17, Coo12, CPAT11, CN12, Dau16, DPK18, DSL15, DPRK12, Di13, DBML16, DSFT17, EAH13, FLCHL10, FBO+11, FNIT16, FSST16, Gag11, Gan14, GWZ+14a, GRCGRRT19, GB10, GS11, GR10, HR13, HS11a, HITU16, HS11c, HEVMSA+19, HM12, Hor13, HMA+18, IFT14, Ish14, JN13, JHSG18, JMX+15, Kap12, KB12, KCDC15, KC18, Kar09, Kar10, Kha16, KCC13, Kit14, Kit15, Kle11, KN15, KK11d, LS17, LSS19, LV19, LSR+13, LCZL15, LHX+19, Lin14, Liu15b, Liu16, LSKM19, LEU+11, Luz11a, Ma14, MC11a, MR12, Mam14, MDC15, MPE15, Mar13, MSC10, MML+16, MPD+10, MQG13, MPL+11, MBBT+12].
VMR11, VVVB10, Vik11a, VOK+18, VO12, WYM15, WR14b, YNL18, YÇO11, YZ13, YW11a, YS13, YH14a, YW16, YLC17, YLYC18, ZS11, ZX12, ZGSM15, ZH15, ZWSF16, ZZC12, ZWE12, ZRLV10, dHLdS12, dSTH17.

quantum [vLRRK15, AGNS14, BMRM19, DMS10, GP13a, SP19, ZBK15].

Quantum-chemical [DLM11, ÖEDB11, Qu13, BF11, DMBL16, DSFT17, MGP16, Ném14, NVPCJ+13, SN15, VOK+18, YNL18, DMS10].

Quantum-chemical-aided [GbZA10].

Quantum-classical [DLM11, ÖEDB11, Qu13, BF11, DMBL16, DSFT17, MGP16, Ném14, NVPCJ+13, SN15, VOK+18, DMS10].

Quantum-matter [Tap15].

quantum-mechanical [LV19, VPFD10].

quantum/classical [CP11].

Quantumness [CD15].

quantum/classical [GbZA10].

Quantum-classical [Cho16, Cho19, Mak15, SPSA11].

Quantum-matter [Tap15].

quartet [HK11, SCZG12, ZG10].

Quartic [VBC+12b, FT15, dAB17].

Quasi [XLLZ10, YZ10, BDPT12, Ho13, KUY16, MPM15].

quasio-classical [XLLZ10, YZ10].

quasi-degenerate [BDPT12].

quasi-diabatic [KUY16].

quasi-exact [Ho13].

quasi-stable [MPM15].

Quinacridone [Gao12].

Quinoline [MLPT10, MAN15].

quinoline-derived [MAN15].

quinolinecarbonitriles [ZFW+13].

Quinone [VWP+18, KSAK17].

Quinone-based [VWP+18].

quintuple [SZS+10, SLZ+11c].

R [DPDR11, DQZF12, GW11, NBL12, Pan16, CPL15, ESS13, GM11, LL17, PCR+11, ZSHL14].

R- [PCR+11].

racemase [LZZ12].

radial [IG11, Kha16, RZ17, SP11, vLRRK15].

radiation [TK16a].

radiative [Ber13a, CCM08, SCZG12].

radical [BLL+13, BAMA12, BRS10, BCS+12, CW+10, GAI19, GKI2, HWH11, IUMVB10, JB11, JAB12, KAR12a, KZA17, KI12, KZZ13b, LCG12, Les12, LLP+13, LSG+14, LV+12b, MM12, OKR12, dMOB12, PM17, RC+19, SSI10, SK14, SSI18, SPSA11, Sch12a, SB16, SLZ+11b, SLZ+11c, SLS+12, SKM11, SWS+14, WLW+14, XM12, YY18a, YSS+10, Zha14, Zha15, ZBL15, ZLW+16, ZJC+13].

Radicals [TWHZ14, IAYL14, Buc12b, CG112, DI11, DFK16, HXX15, KKI4a, KDA+11, LCL+11, LVP12b, MXX18, NP18, RLW+13, RMG+19, SZZ+12, TIN13, TCA10, Wit18, YM11, YL10].

radii [GI10, SV11, TMC+13].

radial [Bar11].

Radu [Tou13].

Quasi- [PL18b].

Ramachandran [MAW+18].

Raman [CK13, NV+13, ČAS13, KV11, LMZY15, PM12, TSFM11, TSBSM12, VFP10, VVS+18, VV12, Y17].

Ramos [COP16].

Randić [AD17, DZ11b].

random [HFBC19, PR10a, Per18, Pog12, SSI12].

randomly [GB10].

Range [BPG+10, AM10, Dun15, GW13, Haj18, IKN13, KAR12a, MJ16b, MIN13, MC18a, RR19, SSK11, SKY+13, ZZ18].

range-determining [IKN13].

range-separated [ZZ18].

Rapid [AA15, NE11].

rare [BAP12, BGL+16, DGL12, JEA13, JMN19, LWL19, MURR13, SZZ+19, TMC18, Y17, ZQC10].

rare-gas [SZZ+19].

Rashba [KV19, SBD+16].

Ratchet [BEFP10].

Rate [WZH13, AFM+10, Buc12a, CAAI12, CGIAI12, DCOC+19, FLCHL10,}
FBM+10, MVC13, MIKH19, NZLG15, dMOB12, ZLWL16, ZXY13, SSP14. 

rates [AC11, CCM08, RFEGPP+16, YK13]. Rational [LLZ+14, WR14b]. 


Rayleigh [BDPT12, MB12, dSCC12]. 

Rayleigh [BDPT12, MB12, dSCC12]. 

RCOOH [DQZF12, NBL12]. RDC [PT13]. RDM [KK14a]. RDX [Jeo18, MJ11, TJS17]. RDX- [Jeo18]. Re [ADR+18]. Reaching [MAN15]. reacting [Gin10]. Reaction [KKH+13, LLM13, MNE+13, OD12, RLW+13, ACMM10, AMMB+18, BRS10, BS14, BAX+19, Buc11b, CdAFS+12, CM12, Chr10, CJGT12, DWJZ11, DAA16, DFK16, EMED+12, EMEPD15, FRNM12, FDMR11, GGZZ16, GB18, HDC+11, HLJZ11, HB14, Hop15, HXX15, HCL31, Kan11, KZZ13b, KMM16, LJK+18, LW11, LLF17, LGW11, LSG+14, MXX18, MIKH19, MAP+10, MBSMJC18, NKWT19, NAK+17, dMOB12, RLW+13, Sch12a, SHS+13, SKM11, SWS+14, TFZ+15, Var14, WLG+11, WLWT12, WZH13, WZ16, XSY10, YS18, ZGSM15, ZXY13, ZQXP17]. 

reactivated [MG10]. reactive [Cho15, dDGNB10, RCM+19, RL12, Srl11b, XCD18]. Reactivities [YM13, LLZZ10, MDNDO+16]. Reactivity [JS18, KSC15, OPF11, PMH+16, TWHZ14, TV13, BVRM10, Cha11, DVC14, DNKCS+12, ESBVJY12, GPFAV9, GTSC+19, GGP13, HMA+19, HR19, Hog13, JW+12, KP10, KO14, MMM12, MUNZVR12, MAP+10, MBA+13, MBBT+12, MBSMJC18, MCRS16, NAK+17, NE11, NZAVR10, OPAVM18,
RGS\textsuperscript{+13}, RBLZ\textsubscript{15}, RBTL\textsubscript{19}, SMGZF\textsubscript{19}, Ser\textsubscript{11a}, SC10\textsubscript{b}, TM19, WJ11, YSK\textsuperscript{+12}, YXM\textsuperscript{+18}, RdA11]. reagent [BPT\textsubscript{12}, LWWZ\textsubscript{13}]. reagents [VOK\textsuperscript{+18}]. Real [GKT\textsuperscript{+12}, HR\textsubscript{13}, Fin\textsubscript{14a}, FNIT\textsubscript{16}, GI11\textsubscript{b}, GI11c, PI16, RLR\textsubscript{13b}, SHKS\textsubscript{15}]. Real-time [HR\textsubscript{13}, FNIT\textsubscript{16}, PI16, SHKS\textsubscript{15}]. realistic [SPSA\textsubscript{11}]. reality [LG10, SDP\textsuperscript{+16}]. Realization [PM12]. really [SMR\textsubscript{14}]. rearrangement [SKS\textsubscript{11}, WTH\textsuperscript{+11}, YY18\textsubscript{b}, ZAE10]. rearrangements [WCGD\textsubscript{12}]. rearranges [MG10]. reason [PWP\textsuperscript{+18}]. ReaxFF [BGKK\textsubscript{16}]. recently [JPPA\textsubscript{10}, TCA\textsubscript{10}]. Receptor [KKM\textsuperscript{+12}, CRSB\textsubscript{12}, CSVCB\textsubscript{12}, MSY\textsuperscript{+12}, SSP\textsuperscript{+17a}, SK11, SKB\textsubscript{18}, WTH\textsuperscript{+11}]. receptors [PRG\textsuperscript{+10}]. recipe [STM\textsubscript{18}]. recognition [AGRI\textsuperscript{+12}, JNY\textsubscript{17}, PvS\textsubscript{10}]. recognitions [YWY\textsuperscript{+12}]. Recognizing [Cav\textsubscript{17}]. recombination [BMF\textsubscript{13}, dMOB\textsubscript{12}]. reconstructed [dLdOdAD\textsubscript{12}]. Reconstructing [YS\textsubscript{13}]. reconstruction [AST\textsubscript{19}, GD\textsubscript{11}]. reconverge [SWS\textsuperscript{+14}]. rectangular [Lun\textsubscript{13a}, Lun\textsubscript{13b}, MPD\textsuperscript{+15}, Tou\textsubscript{13}, YMY\textsuperscript{+13}]. recurrence [HSN\textsubscript{18}]. Recursion [LWY\textsubscript{13}]. recursive [SGH\textsubscript{10}]. reduced [ABLT\textsubscript{11}, CM15, KK\textsubscript{13}, Lat\textsubscript{13}, Per\textsubscript{18}, dCGAM\textsubscript{V2}]. reductase [SDM\textsubscript{12}, SLS\textsuperscript{+10}, TSKN\textsubscript{12}]. reduction [AGOP\textsubscript{18}, Esr\textsubscript{18}, KGK\textsubscript{13}, QCW\textsuperscript{+11}, YHL\textsuperscript{+13}]. reductions [Sri\textsubscript{18}]. reevaluation [GI\textsubscript{14}]. reference [NS\textsubscript{13}, NF\textsubscript{11}, SBK\textsubscript{J18}]. refined [SYK\textsuperscript{+12}]. reflecting [AA\textsubscript{11}]. reformulation [Lev\textsubscript{10}]. refractive [SHMR\textsubscript{11}]. Regina [HS\textsubscript{15}]. regio [CM\textsubscript{12}, GHCM\textsubscript{CMQ\textsubscript{17}}]. regio- [CM\textsubscript{12}]. regio-selectivity [GHCM\textsubscript{CMQ\textsubscript{17}}]. region [EMED\textsuperscript{+12}, KYS\textsubscript{13}, OVT\textsuperscript{+16}]. regional [NGS\textsubscript{11}]. regions [LdBF\textsuperscript{+12}]. regioselective [ku\textsubscript{17}, LK\textsuperscript{+16}]. regioselectivity [DPDR\textsubscript{11}, DMW\textsubscript{Y11}, NAK\textsuperscript{+17}, YNLD\textsubscript{18}, Zha\textsubscript{15}]. regression [VSL\textsuperscript{+15}]. regular [PR\textsubscript{10a}, Pal\textsubscript{10}]. regulated [MBA\textsuperscript{+19}]. rehybridization [Sch\textsubscript{15}]. REIN [MRS\textsubscript{15}]. Reinvestigation [NRH\textsubscript{J11}]. relafen [YN\textsubscript{M13}]. related [Buc\textsubscript{12b}, HNH\textsuperscript{+12}, Kal\textsubscript{18}, Luz\textsubscript{13}, MS\textsubscript{A19}, RALK\textsubscript{18}, RLW\textsuperscript{+13}, SSI\textsuperscript{+10}, TD\textsubscript{11}, TFMC\textsubscript{19}, UMS\textsubscript{13}, VLG\textsubscript{12}, WLWL\textsubscript{14}]. Relation [PM\textsubscript{16}, HSN\textsubscript{18}, KM\textsubscript{12c}, RBGG\textsubscript{M18}]. relations [AE\textsubscript{12}, DB\textsubscript{13a}, GZSM\textsubscript{FN16}, LWY\textsubscript{13}, OOF\textsuperscript{+19}, RS\textsubscript{13}]. Relationship [CZJZ\textsubscript{12}, DNCKCS\textsuperscript{+12}, GXZ\textsuperscript{+14}, Gra\textsubscript{08}, Gra\textsubscript{11}, LBDV\textsubscript{16}, MY\textsubscript{17}, RG\textsubscript{ST\textsubscript{12}}]. Relationships [NBI\textsuperscript{+10}, CJS\textsubscript{NL11}, EKN\textsubscript{10}]. Relative [SFW\textsubscript{12}, BMX\textsuperscript{+19}, LNV\textsuperscript{+18}, MC\textsubscript{17}, Pan\textsubscript{16}, P\textsubscript{SKV\textsubscript{19}, ZSZ\textsubscript{14}]. relatives [Fin\textsubscript{14a}]. Relativistic [BCK\textsubscript{19}, F\textsubscript{12}, Liu\textsubscript{14}, MM\textsubscript{19}, RLT\textsubscript{19}, SH\textsubscript{18a}, CSS\textsubscript{14}, DAC\textsubscript{12}, FSST\textsubscript{16}, GAP\textsubscript{+19b}, Leh\textsubscript{19c}, MCC\textsubscript{GM\textsuperscript{+19}}, M\textsubscript{PTZ\textsubscript{13}, M\textsubscript{ZST\textsubscript{16}, N\textsubscript{SN17}, N\textsubscript{NSSN17}, OCG\textsuperscript{+19}, RR\textsubscript{19}, R\textsubscript{TT\textsubscript{10}, SN\textsubscript{15}, SS\textsubscript{12}, Z\textsubscript{E18}, ZKK\textsubscript{R11}, ZQ\textsubscript{XP\textsubscript{17}}. relaxation [BM\textsubscript{F\textsuperscript{+14}, EBR\textsubscript{11}, FK\textsubscript{L\textsuperscript{+12}, GSP\textsubscript{R19}, Kit\textsubscript{17}, N\textsubscript{g12}, RM\textsubscript{J11}, S\textsubscript{IM14}, YT14, ZP\textsubscript{16}]. relaxed [RS\textsubscript{L10}]. relativity [GSP\textsubscript{R19}]. release [SYK\textsuperscript{+12}]. released [MAP\textsubscript{S18}]. releases [Han\textsubscript{19}]. Relevance [Eng\textsubscript{16}]. relevant [ASHF\textsubscript{13}, KSD\textsubscript{10}, MP\textsubscript{T12}, Wag\textsubscript{14}]. reliable [AB\textsubscript{18}, TKS\textsubscript{K17}].

revisited [DVDBM11, OPC17], Revisiting [DHYC19, GGP13, MJ16a, NS10b, Sha18, VVJ15, VPOG19]. Rg [LL18, BPG+10]. Rh [PP19a, BTH18, BLRD+10, MMR+10, PRPU+13, RW+15, SBB16].


Ricotta [HS15]. ridge [VSL+15]. rigged [IFT13]. right [KBJ17]. rigorous [Mak15, vL13]. Ring [BR08, RB08, AKR+12, AMMB+18, BAX+19, CLXZ12, DLLA10, GZ14, HZW18, KMS+11, KUTS10, LL18, LFP+19, LWL10, LW18, LLVM+13, MSK11, MBSM+18, NHG+12, PCK19, QB15, RLTAT19, Sat11a, TXK+19, WDSL14, WCY+10, YY18b, YTY19, YZ12, YT14, Zha14, BR12a, BR11a], ring-opening [AMMB+18, BAX+19, MBSM+18, TXK+19]. ring-polymer [YT14]. rings [ABTW14, BR08, BR12a, BBKO16, MMM19, RB08, RB11a, RN+12, TKS11, VC13, WvRSW+11, WWD+15]. rippling [MFM18].

RISM [KSS12]. Ritz [DSSM18, MB12, SBM16]. rival [PC16]. Ru [KDOR+17, LL18, SMC18]. RNA [BS14, CLL+11, CAO18, DSVP15, KZA+17, LLLT12, MYZ+10, MMR+10, TD19, ZKWZ17]. Ro [Roy14].

Ro-vibrational [Roy14]. road [HJK14, PP16]. Robust [AAAM12, LY+19]. robustness [Fin14a]. Roby [ABKJ18]. roentgenium [DR18]. Role [BH+18, BR12b, CAPA+18, CM16, HSY+11, PCML08, WLS+19, AM13b, BLWJ17, CG12, CHSO13, DS11, EMK14, ETGLM+19, EMSB15, FBNK17, GbZA10, GLOGM+11, JNY17, KGVG11, KKG12, LSR+10a, LSR+11, LV19, LQ13, MIKH19, MAW+18, MSOV13, MMSC19, Per10a, PWH+12, RMLJ11, SFL+10, SHL+13, SSP14, SC11, SC18, Var14, WCGD12, ZQW+17, ZWE12, dAVdM17, LWL+12, MB12]. roles [JLG+12].


rotamers [HN+12]. rotary [OWD18]. rotating [HRT12, KBG17, Sta10]. rotation [AO12b, CPL15, DDF+12, HK11, HRT12, KBG17, QD10, Sut12]. rotation-vibration [HRT12, QD10]. rotational [AEÖ+12, CCBR+12, DCR10, Puz17, RMJ11, SPO+11, VLM+10]. rotations [JdOS16, KMS+11]. rotovibrational [PBB15]. route


Siroheme-containing [SDM12]. site [AO12a, BGFD14, DLJT14, DPRK12, KRH13, KSY+11, MS10, OH13, PK13a, ŠKB18, SZ11, TOSN12, TSKN12, TYN13, WH18, XCD18, dCDC+11]. sites [ATL+14, BSO11, LKD+16, OPF11, QZH13, RDB18, RDB19, Ser11a, Ser11b, SAC14a]. situation [CPF12]. Six [Nes10, BKKO16].

[CLMY12, GMA+19, HFBC19, LCCH11, LSKM19]. **Solvation**
[GLPA10, MSK+12, RTG+19, AM18, BH10a, Car19, DSM+19b, FAK19, JCC10, Li15, Owe17, PCR+11, RFN+12, SL10, SLS+19]. **solvation-layer**
[RTG+19]. **Solvatochromic** [LCB10, MFB11]. **solvatochromism** [Men15, MR˚A11]. **Solvatofluorochromism** [FSBA12].

**Solvation-layer** [RTG+19]. **Solvatochromic** [LCB10, MFB11]. **solvatochromism** [Men15, MR˚A11]. **Solvatofluorochromism** [FSBA12].

**Solvation** [GLPA10, MSK+12, RTG+19, AM18, BH10a, Car19, DSM+19b, FAK19, JCC10, Li15, Owe17, PCR+11, RFN+12, SL10, SLS+19].

**Solvatochromic** [LCB10, MFB11]. **solvatochromism** [Men15, MR˚A11]. **Solvatofluorochromism** [FSBA12].

**Solvation-layer** [RTG+19]. **Solvatochromic** [LCB10, MFB11]. **solvatochromism** [Men15, MR˚A11]. **Solvatofluorochromism** [FSBA12].
stacked [NMS+10]. stacking
[ACF+11, DB15, FSB16, KdPNNs16, LB18, MHZh18, ZS12]. stacks [FV11].
standard [KGC13, PJP08, Tug13]. State [HXX15, NBZG16, Nic11, ACF+11, Ang10, BPVDB11, BMF13, Bon17, Cao17, CMCN11, Cha11, CJOO11, DGA+13, EMEPD15, FRGC10, FSBA12, GBK18, GSA11, GWZ+14a, GWWH17, GRLA18, GLXL18, Ghu13, GLOGM+11, HM12, HbGqZ17, Ign11, Ign12, IIEH6, IGMK11, JA12, JWJ+12, KAR12a, KYLC19, KY12, Kri13, LSL08, LV12, LJSS12, LDAA11, LZ10, LKd+16, MMP+18a, MFP10, MCC+19, MPT11, MPTZ13, MM13, MML11b, NMS13, OH19, Ped16, PGMR15, Per10b, PMA12, RMJ11, RAGM10, RRCO11, SY10, SFM13, SGC13, SM14b, SS12, SY17, TXK+19, THVP14, TB15, UV18a, VPA11, WKE17, YCH+11, YYX+18, Zak13, ZST+10, ZZ18, PB10]. State- [Nic11]. State-of-the [NBZG16]. State-of-the-art [PB10].
State-to-state [HXX15]. statement [Brä14]. states [Agb12, AM12, Ali19b, ADB10, ARG11, AM15, AY15, Ban12, BG11b, BG11c, Buc11a, Cam10, CR18, CHM+14, CM16, CHSO13, Coo12, Cor16, DM12, DS11, DAR+11, DLRMFY10, DTPC17, DG19, DCHC11, DSSM18, DSSM19, FSK+11, GF12b, GFrdG11, HK11, HGB08, HDF11, HMA+18, JH13, KH10, KT12a, KMF11, Kri14b, Kim16, KGVG11, Kit15, KZ13a, KHH10, KKT13, KKT14, Lad14, LVdSD14, LV16, LCL+10a, LP10b, LCL+11, LGP+11, LGP+12, LGZC15, LDADB+15, MMP15, MMWA11, MT11, MSM16, MQG13, MKD19, MPRB+10, Mor13, MNS11, MB12, NS19, Nal15, NDF10, Nic11, PE11, PSGK17, PRPU+13, Pup11a, RS12a, RAN18, SBM11, SBM16, SF12W, SGG+10, SYL+18, SX+12, SLS+12, SLSZ13, SR11b, SZZ+12, SFY12, SK12h, SCZG12, Swa13, Sza13, TTT13, TÅ10, TBB+19, TD19, VFLG12, VO12, WFS13, WC15, WJL10]. states [XTLA13, XTLA14, ZCG10, Zil14]. Static [CCEGK12, CEFMK12, KA11, MNS11, BL16, FKL+12, FSB16, GH11, IOO18, LXW+12, dWLC14, MA11b].
strained [Iku17, KBJ17]. strains [KK12a]. strategies [GAI19, WR14b].
strategy [BBB+12b, CL08, She12, YZZH15]. strength
[ACL12, BPG+10, CG12, Den19, RB11b, SAC18, WLC+17]. strengths
[BHH+13, MS14c, RTAT19, RB15, ZYL+14]. Stress [LHX+19, Fin14b, GAI19, JMX+15, MPV+11, NIT16, XXJ+16, XWP+18, YXM+18]. stretch
[GPM+15]. stretched [HB14, MJ16b]. stretching [CLXZ12, ZZ15]. strong
[CL11, CSS16, DR18, DLM12, IROW10, RDB19, SRPD16, Sto18, VIk11a, VIk11b, Vik13]. stronger [DI15]. strongly
[Cap16, DM12, Dun15, Jia15, TKN13, WH18]. strontium
[HMI+15, MMR+10, MHO+18, SSP+17a]. Structural
[AGCVG15, CWW+16, DKS11, LZW+15, MPM15, MTHPT12, MFR10, MWC11, MRMA10, QHS11, QCB+10, SBEH11, TCSD12, TCG13, YLW+12, ZHI17, ZCTG18, ART08, AVG19b, CWW+13, DMBL16, DHYC19, EPS+16, GAPK+19a, GKM+18, GMG+11, IAK13, KG17, LLIH15, LZ10, MB14, MSA+12, MA11a, MKHM11, MW15, ORJ18, Pan19, PP19a, PK13b, RJY+10, RNDA+10, TOSN12, TBST10, TFB11, VLG12, WTH+11, WLL+13, WWD+15, YD17, ZWLC12, dSSP19]. Structurally [XxBhD19, DC14b].
Structure [AKHS13, Ber13a, BMBD10, Boc17, CM15, CYL+19, KSG+12, KKT13, LWY11, MMM12, MCARL11, MOY13, MC11a, MTS15, OA13, Owe17, PAK15, SIT+12, TBA13, WU11, YSK+12, AB16b, AEGZ12, AO12a, ACL13, ATS15, BZB13, BL10, BZY18, BG11b, BG11c, Bou11, Bou12a, BDU12, BA13, CLL+11, CZJZ12, CWL+13, CJSNLM11, Cas15, CSVCB12, CJOOW11, DCBB11, DIO12, DVC14, DDS18, DDV12, DMB15, DD17, DG19, DGA+13, DZ012b, DSH+13, Dy16, ETGLMJ+19, ESL19, FLvLA15, FBO+11, Fin14a, Fin15, FBU+11, GBS17, GSZ10, GZ14, GP13b, GEL18, GJ18, GRCATG19, HMI+15, HMA+19, HLMO11, HLLB19, HJ13, IGMK11, IK18, JWG+12, KS11, KK11b, KA13, KK11c, CRK+17, KJ15, KJ16a, KJ16b, KS10, Klee1, KSY+11, KAOB11, KP13, KS18, KOC12, KM19, Lern19, LJYW11, LS19, LLLT12, LZZ+13, Lya14]. structure
[Ma14, MMP+18a, MC11a, MY17, MSG16, MSH13, MPD+15, May14, MBA+13, MPZWD10, MCL11, MGB18, MS14b, MKHM11, MB14, MLC16, NMD+12, PCML08, PT13, PMMGL+11, Puz10, QTCL10, RFN+12, RS12b, RM12, RTGS11, RGST12, RAFR18a, RAFR18b, RMTG11, Rus14, RMY+13, SMK+12, SC12b, SB16, SRS+17, SST011, ScBSR+10, SSW16, SBK18, SCL19, STU19, THT10, TD11, TSH17, TG13, TCPJ+12, VAO14, VLM+10, Ven12, VSS11, VBO+15, WSC+13, WSV10, YAK11, YLW+13, YRN+11, Zha10, dOLdV13, GFB12b, GGD12, NA12]. Structure-dependence [KSG+12]. structure-property [RGST12].
structure-stability [DVC14]. structured [Kim18]. Structures
[CdAFS+12, GLT13, GCD13, IA13, JL12a, KBF+13, LFP+19, LHL+15, MS17, ONK+13, SM16, YWH+12c, ACMRN10, ALK18, ALK19, BMB10, Bra11a, BS016, DWGX12, DM16, GR11, GLF+12, GZ14, GWJ12, HWL16, HWW18, HM10a, JMP19, Kin13, KSSK16, KLYC19, KMM16, Lad14, LL11, LWL+12, MZB+13, MK10a, MLW10, MUNZVR12, MUPC10, MJSC18, MM13, NH18,
NZAVR10, OCGM+19, Puz16, QJ13, SSK+12, SLS+14, SIS+08, SACAI8, SZZZ11, SKY+13, SCZG12, TSKN12, TYN13, TBB+19, VSN+11, WGLX10, WDS19, WJL+10, XTLA13, XTLA14, XWC10, XF19, YJI+13, YZL+10, YZL+11, YZW+15a, YC13, ZLS+10, ZZR+12, ZL12, ZQXP17, dHldS12].

**Structuring** [KRG+13]. studied [AMMK11, BL10, CK17, DCHC11, FBO+11, SJZ+18, TTM16, ZL10, dSdS13b]. Studies [PCF+18, Roy13, ACM10, AVG19b, BD12, Buc11b, CJBMMAPR19, CCA+12, ÇAS13, CYLL11, CTW12, CWB+13, CSSCB12, CSM+12, DSWL11, DSZB18, EAK+10b, EAK+10a, Ef11, For12, GGD12, GKT+12, GZBH15, Hop15, HWL16, JLI12b, KDC12, KMM+18, KA13, KSY+11, KAOB11, LSL12, LSR+13, LBY+14, LGZC15, LWJL10, MANP17, MLPT10, MMM+12, MSAB19, NTCK13, ONBP11, ÖEDB11, PBM10, PTD12, PETB18, PAPCM+16, RJA+10, RGT11, RndA+10, Ric11, Rgs+13, RGR12, Roy14, SMK+12, SD16a, SC12a, SJZL12, SIS+08, SK12b, SZ15, SSB+12b, TIKN11, TOSN12, TYN13, TAY11, Tan12, TIN13, TSL10, TSHR13, UJSJ13, WGLX11, Wan13, WZM+13, WYWL13, WHM14, Wit18, WWGW18, XS18, XFW+14, YZL+10, YZW+15a, YB11, ZZL+11, ZZX10, ZYZ+11, ZQJW13, ZLY+14].

studies [ZWL18, ZSZ14, dAGNJT12, YWY+12]. Study [Bar11, BWB+18, CH17, CYL+18, IFT13, IFT14, SGL+16, SS19b, ZCP11, AC19, AFC+10, IAY14, AM12, AASU+17, AEAS+19, ATM17, AKC10, ASW13, AVG19a, ASD14, AMAC12, AG19, BMK+14, BD14, BF11, BCGC12, BDF+16, BDF+18, Bas11, BAMA12, BLB+18, BLR12, BS11, BEN11, BZH13, Ber13a, BL11, BLRdA+10, BHAH+18, BS14, BSSS19, BZ15, yBZC18, BXZ+19, BGD17, BLDv19, BMF13, Bon17, BGJS+18, BDR12, BCF+11, BPSM12, BLM+12, BJ17, BddMAV12, BTH18, Buc10, BO11, BVRM10, BCS+12, BB16, BSV12, BSPK11, CRB+12, CM13, CAX+11, CLXZ12, CCL+13, Cao17, CPL15, CPF12, CBFR+12, CHM+14, CHI+19, CG12, CW16, CM12, CCL+10, Che12, CCS13, CWW+16, CZL17, CLY12, CS13, CWS15, CZCW19, CK13, CFGC11, CGIA12, CAPI12, CPAT11, CJOOW11, CD12, CS18, DWJZ11, DCBB11, DIOG12]. study [DMAB12, DAR+11, DSD18, DKS11, DP18, DS12, DCDD10, DSRGD12, DPRK12, DPDR11, DTEMK11, DZ11a, DLO16, DG19, DMS+10, DCdG10, DDF+12, DdG+11, DQZF12, DWGX12, DS+13, DCR10, DSFT17, DFF+13, EG10, ESDO16, ELCO8, EAH13, EO11, ETGLMJ+19, EBH11, EA12, ENV15, ES17, ESR18, EM19, EBVJY12, FSO+11, FZ18, FF10, FO10, FM16, FTB11, FRNM12, FDR10, Fin14a, FT15, FPRGMHGB12, FBU+11, Gag11, GBS17, GWM11, Gao12, GLF+12, GGJD13, GZW16, GGF12, GKL12, GLXL18, GIO12, GFB21b, GC18, GP13b, GMT16, GMT18, GS11, GLOG+11, GHCMCMQ17, GB18, GWME18, GD11, GSB10, GT13, GTSC+19, GGP13, GLPA10, GCZ+14, HNH+12, HMA+19, HK11, HDS+11, HJLZ11, HZL+14, HZL+19, HDF11, HHL12a, HHL14, HM12, HM10a, HK11, HZZW11, HFL+17, HHL+12b, HgQZ017, IIV+11, Iku17,
study [IM15, JPPA10, JN13, Jnl10, JL10, Jn10, Jbl18, JS17, JCCZ12, JSLH14, JLL17, JB11, JW1+2, JFDD10, KM12a, KS11, KWC10, KWC11, KP11, KBF+13, KKM+12, KI15, KI12, KK14b, KS11a, KZZ13a, KZZ13b, KUTS10, KKT13, KKT14, KG08, KO12, KMU+13, KK11d, KBMM10, Lan10, LFF+12, LGM+18, LLM13, LKOS17, LJK+18, LDSD14, LPOP12, LZB10, LCL+11, LJJ+11, LW11, LW1+11, LW1+11, LDP+11, LDP+12, LDP+13, LWX+14, LLL16, LRY+17, LLF17, LD17, LZW+18, LLT18, LFTL18, LLIW+11, LLIL+11, LGW11, LCZ15, LL19, LCCH10, LLLZ10, LCCH11, LSS12, LXW+12, LWZ+14, LL17, LLW+12, Lu10, LWC+10, LCS+11a, LCH+11, LCS+11b, LXL11, LLB13, LW13, DVMC19, LKZ+16, LMY+10, MLW+14, Ma14, MY17, MAD12, MBK19, MSG16, MZB+13, MF11, MK10b, MK12, MLC+11, MCP10, MMR+10, MCC12, MVG18, MP12, MTL+12, MSC10, MWW19, MOY13, MMWA11, MMC+19, MUNZVR12, study [MUPC10, MDND0+16, Men10, MFZ+18, MCL11, MKSG13, MS17, MHHP1+17, MM11, MSK+12, MPL+11, MGD11, MTS15, MPREG12, MMRA10, MML+11a, MLB+12, MBBT+12, Mor11, MM13, MG10, MMF+13, MSR+11, MSOV13, MCIS16, MOH+12, ND11, NS10a, NHG+12, NDH10, NBL12, NAK+17, NTL10, NL11, NFQ+11, NH12, NRS11, NRS+11, NPR+11, NRJH11, NJA+12, NIT16, NVA11, NOV15, OAC17, OCP17, OAA19, OH12, OH13, OCB+10, OPP+14, OMD13a, OM13b, OD12, ODL16, POL12, PS13a, PE12, PTS+11, PWP+18, PDC14, PHE+16, PE11, PWL+10, PSK19, PK13b, PKK14, PRG+10, PAD+10, PRP+13, PM17, Puz10, QHS11, QCW+12, Qu13, RYMI12, RFN+12, RGPZD13, RRVJ10, RS12b, RSN12, RSM12, RCM+19, RD14, RRR19, RST12, RDB19, RYW+15, R19, RCM10, RJLPGH+13, RDM+11, RBVAG18, RNE10, RNB+10]. study
[RS11b, RRB12, SF13, SB11, SB19, SIT+12, SK14, SD16b, SBE11, SSK11, SVRG12, SB10a, SKHN13, Sat11b, Sch12a, SK17b, Ser11a, Ser11b, SLS+14, SK11, SHL+13, SLS13, SHE10, Shi13, Shi18, SL10, SKM11, SM13, SR13, SSTD11, SLA12, SK11, SR18, SSA18, SSP+17b, SB18, SMA11, SZ11, SBB15, SZZ11, SZ12, SLZH12, SHW+13, SRI18, SMGZ13, SK10, ST19, SYQ+10, SW12, SWS+14, S1L+14, SGL19, SYY16, SCZH16, SS13, TK16a, TV13, Tav11, Tav12, TM13, TTO10, TDO17, TU10, TYL10, TSL11, TFF+15, TJS17, TFA10, TSH17, TFB11, TC110, TGA+11, Tug13, TWR15, TPT+13, TPT19, UKF+11, UMS13, VF13b, VPJC12, VFSC17, Var11, VHTK15, VNN+16, VLM+10, Ven12, VSMK13, VSMK15, VV12, VV13, Vie17, Vi13, VFK+19, VDG13, VS19, VO11]. study [VO12, WML10, WXZ+11, WJL+11, Wan11, WvRSW+11, WLL11, WL11, WL11, WLWT12, WLZ+12a, WLZ+12b, WWHZ13, WSH+13, WHY+14, WY15, WTW+15, WD17, WWQ17, WG18, WZZL10, W1Z+11, WWX+11, WLD+10, Wu11, WSL+11, WZC+12, WRW+18, XNL+14, XX12, XSL12, XGH18a, XLL10, XZCH11, XZ11, XWC11b, XG+18b, Y12, YM13, YNLD10, YY15, YY18a, YY18b, YZL+11, YZJ15, YJ12, YZZ16,
YLZ$^{+17}$, YZ$^{10}$, ZKKR$^{11}$, ZSAP$^{11}$, ZSASS$^{13}$, ZAE$^{10}$, ZLR$^{15}$, ZRGE$^{+19}$, ZWWY$^{10}$, Zha$^{10}$, ZLS$^{10}$, ZZW$^{11}$, ZLZ$^{+14}$, Zha$^{14}$, Zha$^{15}$, ZLWL$^{16}$, ZCX$^{+16}$, ZKZW$^{17}$, ZBG$^{+19}$, ZSO$^{+10}$, ZRR$^{+11}$, ZPB$^{12}$, ZSS$^{+13}$, ZLWZ$^{16}$, ZTC$^{11}$, ZQXP$^{17}$, ZLY$^{+14}$, ZPW$^{16}$, ZBBB$^{17}$, ZDZL$^{11}$, dSdSPG$^{11}$, dSdS$^{13a}$, dLRR$^{11}$, dOR$^{10}$, dOdONM$^{12}$, dLIAI$^{12}$, BVP$^{13}$, SW$^{12}$. **Sturmian** [FRGC$^{10}$, SS$^{12}$]. **stryrene** [DPDR$^{11}$, MCC$^{13b}$]. **styryl** [TPT$^{19}$]. **styryl-bodipy** [TPT$^{19}$]. **styrylnaphthalene** [Bud$^{12}$]. **styrylnaphthalenes** [BO$^{11}$]. **subcluster** [ALA$^{15}$]. **subgroup** [BSPK$^{11}$]. **subphthalocyanines** [PZ$^{19}$]. **subsidiary** [LWY$^{13}$]. **Subspace** [TG$^{16}$]. **subspaces** [TLC$^{+17}$]. **Substituent** [BHMN$^{19}$, EHKD$^{11}$, EEMSS$^{14}$, MKHM$^{11}$, RY$^{12}$, YRN$^{11}$, dSNBG$^{08}$, DWZZ$^{15}$, EAV$^{16}$, JNY$^{17}$, Val$^{17}$, XX$^{12}$, ZBG$^{+19}$, ZYL$^{+13}$, ZBBB$^{17}$]. **substituents** [AG$^{10a}$, AMK$^{10}$, KMM$^{+18}$, LZZ$^{+17}$, SN$^{11}$, WDS$^{19}$, WLC$^{+17}$]. **substituted** [AAA$^{12}$, ASD$^{18}$, BG$^{13}$, CLXZ$^{12}$, EHGD$^{11}$, EKDI$^{2}$, IGMK$^{11}$, IUMV$^{10}$, JLL$^{11}$, KMMS$^{17}$, ILBQ$^{+19}$, MXC$^{18}$, NAK$^{+17}$, NZAVR$^{10}$, PS$^{13a}$, PF$^{19b}$, PSK$^{+13}$, RLTA$^{19}$, SSKS$^{12}$, SN$^{12}$, SMGZ$^{13}$, SZL$^{+14}$, SC$^{18}$, TT$^{10}$, Tig$^{13}$, VSN$^{+11}$, ZLY$^{+14}$]. **Substitution** [SPIL$^{14}$, Buc$^{10}$, Buc$^{11a}$, Buc$^{11b}$, EMS$^{16}$, HLJZ$^{11}$, JLG$^{+12}$, ND$^{10}$, RFR$^{+12}$, Ril$^{10}$, RB$^{11b}$, dAB$^{17}$]. **Substitutional** [BSO$^{11}$, KSS$^{19}$]. **Substrates** [dSSdSGA$^{12}$, FBD$^{13}$]. **subsystem** [MA$^{10}$, NS$^{10b}$, Sha$^{11a}$, YKN$^{13}$, ZS$^{11}$]. **subsystems** [GHP$^{11}$, HS$^{11c}$]. **subunits** [Sch$^{15}$]. **subvalence** [dCDC$^{+11}$]. **Successes** [Swa$^{13}$]. **successive** [SM$^{14b}$]. **such** [Ser$^{11a}$]. **sudden** [CLXD$^{15}$]. **suddenly** [MAPS$^{18}$]. **sufficiently** [MK$^{10a}$]. **sugar** [BS$^{14}$, SKM$^{11}$]. **sulfate** [CAPL$^{12}$, FMP$^{+17}$]. **sulfate-methane** [CAPL$^{12}$]. **sulfated** [MC$^{16}$]. **sulfenate** [ZAE$^{10}$]. **sulfide** [BAP$^{13}$, DWJZ$^{11}$, JAB$^{12}$, MA$^{11a}$, MTS$^{15}$, SSP$^{14}$, TCSD$^{12}$, YGLL$^{10}$, YLZ$^{+17}$]. **sulfinyl** [SFW$^{12}$]. **sulfite** [SDM$^{12}$, SBSD$^{18}$]. **sulfonamide** [TPdMB$^{12}$]. **sulfoxide** [LdBF$^{+12}$, ZAE$^{10}$]. **sulfur** [CK$^{17}$, DI$^{11}$, DSFT$^{17}$, GFRG$^{G1}$, GCD$^{13}$, KM$^{19}$, LD$^{+16}$, NFD$^{+10}$, NFO$^{+11}$, Oni$^{12}$, SFW$^{12}$, SCB$^{+14}$, dLdOdAD$^{12}$]. **sulfur-containing** [NFD$^{+10}$]. **sulfur/selenium** [KM$^{19}$]. **Sulfuric** [dLdOdAD$^{12}$]. **sulphonamides** [EAK$^{+10a}$]. **sulphuric** [SMRK$^{18}$]. **sumanene** [ONK$^{+13}$]. **Sup** [LJ$^{16}$]. **super** [Man$^{16}$, MBSAG$^{16a}$, MBSAG$^{16b}$]. **super-resolution** [Man$^{16}$, MBSAG$^{16a}$, MBSAG$^{16b}$]. **Superacidity** [VV$^{18}$]. **superacids** [CS$^{18}$, Val$^{17}$]. **superalkali** [TL$^{15}$, WCY$^{+10}$]. **superalkalis** [STM$^{18}$, Sri$^{18}$]. **superatom** [JHL$^{+18}$, YLWR$^{L12}$]. **Superatomic** [MCK$^{17}$, GAPK$^{19b}$, MC$^{18b}$, TFCM$^{19}$]. **superatoms** [GAPK$^{+19b}$, TFC$^{19}$, TF$^{B11}$]. **superbases** [CT$^{14}$]. **supercomputers** [CLK$^{15}$]. **supercomputing** [GE$^{12a}$]. **Superconductivity** [DB$^{13b}$, LAR$^{10}$, BCP$^{10}$, Dum$^{15}$, MC$^{14}$, SM$^{10a}$]. **superconductor** [HKIH$^{13}$]. **superconductors** [GdLT$^{12}$, PK$^{13b}$]. **supercritical** [BBB$^{+12b}$, Ma$^{14}$]. **superfluidity** [ZLR$^{15}$]. **Superhalogen** [SM$^{18}$, SR$^{13}$, Sk$^{18}$, SM$^{14b}$, SM$^{14d}$, SM$^{14c}$]. **Superhalogen-supported**
DMAB12, DLRMFY10, DBTA19, DCDD10, DI18, Dun15, DB15, Fer19, Fin16b, FSST16, GB10, HS11a, HITU16, HFdGC14, HKLW13, IFT14, JE10, KH12, KK13, Kha16, KCC13, KSD10, KSN+10, KYH+13b, Kon11, Kry11b, Kry12b, KM19, Lad14, LS17, IV16, LGZC15, LC19, LRMAA19, LZD+11, LNI12, MCGG+19, MMM19, MANP17, MNP19, MC11b, MSAB19, Nag16b, NKF+13, NDH00, Nas19, NGS11, NYS+10, NMV+14, OPC17, Per10a, PBB15, QTCL10, RB08, RB11a, RAMB18, RAGM10, Roy15, RS13, SLG11, SBAT16, SK11, SMV11, SK17b, SKLC19, SKS15, Sko16, SKV12, SMMT13, SBSD18, Swa13, TFSRM11, Tok16, TRZ+19, systems [VOAH18, WCM14, XTLA13, XTLA14, YYI+12, YWH12a, YWH12b, YFY17, Zak16, ZWE12, dGR14, dOR10].

systems* [Mam14].

Szeged [Tra19].

T [BL12, BTH18, CPF+11, SLS+11, ZHL+19, GWMI11, WLL+13, BBM17, BTH18, SD13c, XLLZ10, YGLL10, dOR10].

t-cell [WLL+13].

t-junction [SD13c].

T4 [DFF+13].

table [Gar08, GI10, Kut10].

Tables [Rus14].

TACA [Kao11a].

tailed [GbZA10].

tailoring [AV19, BHAH+18, MMA10].

take [PUGSFM18].

tame [DB13a].

tardy [FK18].

target [HM10b].

targets [PUH+11].

tartaric [LCZL11].

Tautomeric [SOM10, CCL+10, JN13, LDW+11, NJA+12, TSH17].

tautomerism [HS11b, PS13a, VF13b].

Tautomeric [SOM10, CCL+10, JN13, LDW+11, NRS+11, NJA+12, TSH17].

Tautomer [PJP08].

Tea [MKHM11].

Technical [MMP11].

tactic [KdSM+10, LKJ13, MJSC18, SR12, SOF+10].

Techniques [DW12, LSR+10a, LSR+11, MQG13, OS11b, RW11, SKV12].

Technology [YSA+11].

Tell [DMAB12, AGPDZ13, DMAB12, GB12a, HR12, HFZ12, JZP17, RGPZD13, SBD+16, TPCJ+12, WLZ18, YY1+13, ZFC12].

Teller/Renner [DMAB12].

telluride [KG08, MW15].

tellurium [ESDO16, RR19].

tellurium-containing [RR19].

temozolomide [KdPNNS16, KMMS17].

Temperature [Buc12a, GFPAV19, KKH+13, MKSG13, PMMG+11, Boc12, CAAl2, CS17, Dun15, KAR12a, ILBqD+19, LL19, MOH+12, Nag17, TD11, WCGD12, ÁFV12].

Temperature-dependent [GFPAV19, ILBqD+19].

Temperature-programmed [ÁFV12].

Temperatures [Chu12, STM17].

tendencies [SMP10].

Tensor [SPM+15, BL19, Fin14b, JMX+15, LHX+19, Lya14, NIT16, XXJ+16, XWP+18, YXM+18].

Tensorial [SD13c].

tentative [YFY17].

terephthalate [TIN13].

term [IIH16, OS11b, ZLJ11].

terminal
Theoretical
[Zhao10, ZZX10, ZLLS10, ZYZ11, ZZR12, ZSHL14, Zha14, ZQW17, ZYSW17, ZSO10, ZFS11, ZL12, ZSS13, ZTC11, dSDPG11, dARAV12, dOdNM12, AZD11, ASD14, AG19, BLL13, BLRD10, BG13, yBZC18, BPSM12, Bu10, CZJZ12, Cao17, CHH19, CG12, CYLL11, Che12, CHL14, CZCW19, CGIAI12, CPAT11, DDY12, DPRK12, DTEMK11, DZ11a, DQZF12, DC12, EI11, EMED12, ENV15, FMP17, Fri12, GLF12, GHG12, GLXL18, GT13, GGP13, HYZ13, HSS18, IHk17, Jia10, Jia15, KO14, Kim16, KC19b, KO12, LS17, LRP11, LL11, LS19, LCZ15, LMC19, LZ12, LS19, NBL12, N`em14, NRS11, OKR12, OAA19, OH12, OH13, OMD13a, ORJ18, POLV12, PM17, Pu10, RGR12, SF13].

Theoretical/computational
[SA18, SFL10, SSK10, SIS10, SACA18, SRA11, SYQ10, Tch16, TK16b, VATPR11, VFCSC17, VLM10, VSMK13, VFK19, VO11, WGL10, Wan11, WLZ12a, WZM13, WWB14, XF19, YM12, YZ15, YLW13, ZAE10, ZWWY10, ZR13, ZKW17, ZPB12, ZW15, ZLW16, ZMB17, dLRR11, dOR11, dMCUMdLR11, DJB10, DC10, HHL14, LEU11, S15].

Theoretical/computational
[N`em14].

theoretically
[An13-49, BHA19, Buc12b, DZ17, HKL13, ISN13, IKN13, Koc13b, Kri13, Kut13, LM15, MIN13, NS13, SS10, S13, SY10, SK15, TH13, YSS10, Y13, Y14, AC19, AB19, AM13b, AgPD13, BV13, BAX19, BGV12, BK11, BJdMAV12, Cam12, CCL13, Car19, CEFK12, Cha11, CH12, CL12, CZLD17, C19, CK17, CF14, CTD10, CST16, DW11, DKB11, DSS10, DM10, DRY10, E10, F10, G10, GPP19, GCK17, GM11, GEL18, GS11, GCZ14, HMA19, HRR19, LL14, HZZ19, HMA18, IN15, JROW10, JR12, JPP11, HS18, JMX15, JW18, KARI2a, KC15, KC18, KAR13, KKL16, KS17, Kit14, KM12c, KYLC19, KdSM10, KJ14, KMT13, KJ18, KLE19, Lar12, Lat13].

theory
[LPO12, LCL10b, LW11, LW12, LP12, LBY14, LHX19, LLW11, Lin14, LDZ16, LL12, Ly14, LKd16, MYZ10, MLW14, MJ16a, Mam14, ML11, MFK12, Mas14, MW16, MLK17, MLB12, MBBT12,
Mor13, MJM19, MCRS16, Mur12, Nag15, Nag17, NSN17, NNSN17, Na13, NS10b, NAK+17, TTN10, NL11, NMIP14, OK16, OD16, PS10b, PS14, PK13a, PABSK16, PP16, Pat15, PTH11, PR10b, PBB15, PU14, PM16, PJP10, PMAP12, PI16, PC13, QBRA18, RGPZD13, RCM+19, RB18, RMG+19, RMC19, RAMB18, RS09, RS11a, Rud12, SVRGV12, SLC+18, SN15, SN12, Sha18, SZS+10, SLZ+11c, SLS+11, SHL+13, SJZ+18, SM12, Sto18, SK12b, SD13c, SS13, TFBG14, TIN13, Tan13, TTD13, TH12, TDOD17, TG16, TXK+19, TLC+17, UV18a, VPGC12, Var11, VUC13, VBO+15, WKE17, WJL, WW11, WJY15, WB17, WDJ+17, WTZ+11. **theory** [Wit18, XNL+14, XGH+18b, YKM+15, YLH+19, YWH12a, YWH12b, ZS11, ZQCJ10, ZLWY13, ZCX+16, ZBG+19, ZMZ13, ZSZ14, ZZ18, Zho18, dCSDdMC13, dSTH17, BM10, SP19]. **theory-based** [KSAK17, WJY15]. **there** [GI11f, SMR14, TKSK17]. **Thermal** [CEV10, FBM+10, NG11, AFM+10, AMMB+18, Chu12, Liu15a, MVC13, MCC12, Mar13, MOSK10, MML+11a, MB13, PP19b, RRRV19, YZ13]. **thermalization** [Nes11], **thermally** [PFdM13]. **Thermodynamic** [Nag17], **thermoelectric** [KG17], **Thermochromie** [Kim19, Rus14]. **Thermochemistry** [ABTW14, ÇBAT16, AK11, BYAT13, ÇT14, HZG12, Rus14, WZX15b], **Thermodynamic** [JAB12, VOAH18, XNL+14, COCF+14, DWGX12, Kim13, LZZ+13, OSJ+12, Pan19, PP19a, RMLPGGH16, Tav11, TSH17, dOLdlV13]. **Thermodynamical** [Nag17]. **Thermodynamics** [MLW16, PK16, BvWG14, Bra19, DP11, PD11, PRFR17, RTG+19, WSC11]. **thermoelectric** [KG17], **thermostats** [GVPCK10], **third** [KWC11, MMF+13, NKF+13, RS09, RS11a, WLZ+12a]. **third-body** [KN15, Lev16]. **Thoughts** [DJ18, FMD+19]. **Three** [DMS+10, FMMD+10, HYH+10, Kry10, LQZ12, MPD+15, MMP+18b, RAN18, ARG11, Buc10, Buc11a, CG12, GSaY11, Hog13, KV19, LWY13, Mat02, Mat10, MUPC10, RZSZ18, RAGM10, SD13b, SYL+18, SKY+13, WvRSW+11, WLZ+12b, Zha14, JA12]. **Three-body**
trans [BM+]\textsuperscript{15}, Bud\textsubscript{12}, CCL\textsuperscript{+10}, FMKJ14, KZZ13b, MB13, XZ11, GLOGM\textsuperscript{+11}, LCB10]. trans-

trans-3 [MB13]. trans-diarylethylenes [Bud\textsubscript{12}]. trans-isomers [FMKJ14]. trans-RuCl [CCL\textsuperscript{+10}]. trans-to-cis [Bud\textsubscript{12}]. transcriptase [SKHN13]. transcription [Nag17]. transesterification [GCZ\textsuperscript{+14}, MCRS16].

Transfer [SS10, AKC10, ARH\textsuperscript{+13}, BSS16, CS17, DS11, DAA16, FV11, FDMR11, FSBA12, GI1\textsubscript{a}, GHCMCMQ17, JdL08, KyH13a, KUS19, KAOB11, KT12b, KBMM10, LZZ12, LYS\textsuperscript{+19}, LYL\textsuperscript{+12}, Lu10, MANP17, MPE15, MHOG18, MNC12, NMS\textsuperscript{+10}, NBZG16, OK19, QJ13, RY12, RS12a, SSK11, SMRK18, Sch15, SHS\textsuperscript{+13}, SCS15, Tav11, Tav12, TCG13, WJ11, XDM\textsuperscript{+10}, YH14b, Zen11, ZZ18, ZB18, dA12, dCDC\textsuperscript{+11}].

transfer/induction [dCDC\textsuperscript{+11}]. Transferability [GSR12, STM17, RLER10]. transferred [HSN18]. transfers [KyH13a, YYS15, YY18a]. transform [SFY12, YSO\textsubscript{12}]. transformation [DMAB12, DM12, DK13, HHYC\textsuperscript{+18}, IM15, Jør15, Jør18, Mam13, Rua10, SN15, TSS\textsuperscript{+15}]. transformed [Hor13]. transistors [SAHAA16].

Transition [BLdV19, Pie11, ALK18, BEM11, BZBZ13, Ber13a, BVP14, BB10, BDR12, Buc11a, BN11, CWW\textsuperscript{+16}, Cho16, Cho19, CP13, Dau16, DMS\textsuperscript{+10}, DMBL16, EMED\textsuperscript{+12}, EMEPD15, GRLA18, GFB12b, GM11, GZBH18, JHL\textsuperscript{+18}, KWC11, Kin13, Kry12c, Lar12, LCB10, LKd\textsuperscript{+16}, MKM11, NKWT19, NZ13, Qu13, RZC13, SDS19, SFW12, SAHG11, TMC\textsuperscript{+13}, TTD13, VSMK13, VO12, WWC17, WR15, ZK12, ZFC\textsuperscript{+17}, ZHI17, ZSZ14, Zil14, KAR12a].

transition-metal [GZBH18, TTD13, WR15]. transition-metal-doped [RZC13]. transition-metal-like [JHL\textsuperscript{+18}]. transitions [AC11, BCNR18, BTH18, CK13, GC19, ILBqD\textsuperscript{+19}, LZ10, MS12, MLDP10, JP08, SLC\textsuperscript{+18}, VV12, VV13, Zen11]. Translation [RLER13b, Laz14].

translational [Lad14, Tou11b, XTLA13, XTLA14]. translations [Hog10]. transmembrane [KMT\textsuperscript{+12}]. Transmission [RBGG18, CDT12, NTCG18, NA12, SD13c]. transmitted [Cho15].

Transport [Yam11, DCZ17, DLZ11, ETGLMJ\textsuperscript{+19}, Gao12, Jan10, JR19, KM12c, MSG16, MMP11, OH12, OH13, PFdM13, RBGG18, RRRV19, SSKS12, SSB12a, WDS19, ZYZ\textsuperscript{+11}, ZQJW13, ZY13, ZB18]. transporting [MCL11]. Trap [YZZH15]. trapped [TG13]. Trapping [PDNC14, LL18].


trichelates [LOHB13]. trichloroacetyl [SKS11]. tricks [SCB\textsuperscript{+14}]. tricyclic [ZWZK19]. tridiagonal [HFZ12]. tridiagonalization [ZHF12]. triel

U [BB10, OGvSG18, WDJ17]. UB3LYP [YSK12]. UBD [NYS10].
UV [AFC+10, BSS15, Bou12b, ÇAS13, SDS18, FPRGMHGB12, MSBF18, PJ08, PJP10]. UV-Vis [DS18]. UV-visible [Bou12b]. UV/VIS [PJP10, PJP08]. uvarovite [MPZWD10, VPFD10].


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vancomycin [LSR10b]. vancomycin-group [LSR10b]. van’t [Buc10].

Variation [JWG+12]. Variational [FAFR12, CDS+18, DSS18, Kri13, NS10b, Oht13, dMOB12, SBM16, SSB12a, Sha11a, ZS11, MHT+08]. variations [KBGC12, MB12]. variety [AM10, TOSN12]. Various [MGK+12, ART08, HFL+17]. VASP [WMK+19]. vdW [KMNSP19]. vdW-TSSCDS [KMNSP19].

vector [AMMB+18, HEVMSA+19]. vector-based [AMMB+18, HAX+18, JMXT+15]. vegetable [PWM+12].


versions [ND10]. Versus [FKBG19, AM18, CAPGAIG18, CLMY12, DI15, DLP17, FLCHL10, GKM18, HYZ12, HYZ19, KyH13a, KUt13, LJK+18, MMF+13, SALK19, SL10, VMC11]. vertex [FSQ+11, GAPK+19a, SALK19]. Vertical [ABG12, GMA+19]. SLC+18, SOM10]. vertices [BBKO16]. very [QBRA18].

VI [Lu10]. via [BGL+16, BLKB11, CHH+19, CS17, Dw13, DMWY11, DWZ15, Gan14, GLX18, JHS18, KZA+17, LCK+16, MB12, MCMS16, OPC17, Ols11b, PR10a, PM12, PM16, SGB11, SLC+18, SRA+11, TGRP19, YSÖ12, Eng16].

Viable [FXxBlD19]. vibration [HK11, HRT12, KBG17, LZW+15]. QD10, SPO+11]. vibration-rotational [SPO+11]. Vibrational [AC12, CTVA12, Cybi11, FKL+12, KKT13, KKT14, SD12, AF19a, AGCVG15, BBB+12a, BB16, CP10, DK13, DCFD10, DWG12, For12, FKC12, dDGN10, HH18, Ish14, KLi11, LJW+11, LWWZ13, MC11a, MBKH19, MCE11, MB14, MMCN+11, NDM+12, PM12, PBB15, RPBB11, RSM12, RCI11, Roy14, SBAT16, SA11a, SPO+11, SZZZ11, SLZ+14, TU10, Tou11a, WHY+14, YWH+12c, ZGSM15, ZPZ15, ZQXP17]. vibrationally [LMZY15]. vibrations
Ano18-28, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18o, Ano18p, Ano18q, Ano19a, Ano19b, Ano19c, Ano19d, Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j, Ano19k, Ano19l, Ano19m, Ano19n, Ano19o, Ano19p, Ano19q.

Volume [Ano19r, Ano19s, Ano12o]. vortex [GKS10].

torticity [BL19, HMH10a]. vs [Ali19b, DG19, SP19, Yam10]. VSc [BBYZ18]. V [LW18].

vsLab [CRFR11]. W [HNBS18, MLY+16, ZLY+14, GAPK+19b, SX5+12]. W1BD [VF13a].

W [OK16]. W2w [OKR12]. Waals [BPG+10, BAP12, Ber13b, GRCATG19, KKL+16, NRSK16, PABSK16, SZZ+19].

waistline [TMC+13]. walks [PR10a]. wall [DI10, SD13a, TC10]. walled [Bas11, ETGLMJ+19, HNBG15, KG08, MSOV13, SD16a]. walls [RBVAG18].

Wannier [PABSK16]. warm [DW12, Ng12]. Watch [ZLWY13]. Water [Kim18, RFEGPP+16, WW11, XZM+12, AF16, ATS15, BBB+12b, BPSM12, BCS+12, Cha10, CNSK11, Chu12, CK17, CAPL12, DPK18, DE18, EFO11, EO11, FMCA11, FUE+12, GZ10, GLPA10, HQ13, HS11b, KK11c, KV11, LLF+12, LMM13, LJW+11, LNGW14, LCB10, MA14, MAD12, MFB11, MK10a, MKE10b, ME15, Mar12, MTL+12, MPV+11, MOE+11, MD11, MRA11, NS10a, OHDA13, OD12, PW10, PCMG12, QSLY10, RRVJ10, RAK10, SYK+12, SSS+12, SMEH15, SMEH16, SK12a, SJZ+18, SL10, SCL19, SW12, SJW13, SHMR11, TGGP19, Var14, WCGD12, WWD+15, WTP+19, WSV10, XS18, XGH18a, YY18a, YY18b, YT14, ZKZW17, Zai13].


Wave [AB16a, HDOS12, Kut13, NS13, TKN13, TH13, YKN13, Bae16, BR12b, CW13b, Cho19, CSMZ10, D'y16, GBS17, Gao11, GKT+12, HR12, Hog13, IK18, KRC+16, KH10, Kar13, NT13, OHDA13, OH19, RZ17, RW11, SSAM13, SGG17, Tob19, WC14, WH12, YLYC18, ZHF12, ZCG+17].

Wave-function-based [AB16a]. wave-functions [Hog13]. wave-packet [Bae16]. wavefunction [CH17, DAC11, GWHH17, ZWSF16].

wavefunctions [AC12, Lai11, Yur13, Yur15]. wavelengths [JdOS16].

Wavelet [SFY12, GSPR19]. wavepacket [GWZ+14a, HKZZ15, Han19].


withdrawing [BSSS19, KPL+17]. within


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