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**Title word cross-reference**

(001) [dLdOdAD12]. (100) [MFK+12]. (1 ≤ n ≤ 6) [UDVD10]. (2 ≤ n ≤ 8) [BLRdA+10]. (A = N, B) [ASW13]. (m + n = 3) [UKF+11]. (m = 5, n = 2) [MHHRP+17]. (m = 6, n = 3) [MHHRP+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]. (φ - ψ) [MAW+18]. + [Buc12a, CdAFS+12, DMAB12, FRNM12, GKT+12, KT12b, LWWZ13, MEEA+13, MPRCEG12, MOH+12, RSN12, SABA+12, SD12, WZH13, XLZ+12, YGL+11, YZ10, ZH12]. 1 [BEM12, DFK16]. 1/3 [KLZQ15]. 13 [LXD13]. 14 [YD17]. 18 [YD17]. 13\(^1\)M\(\nu\) [GWZ+14a]. 2 [ABTW14, CPL15, HGB08, IK14, LLZaH14, LD17, NF11, SPD+18, SsdS17, YSW11]. 2n + 2π [MB13]. 2n = 68, 70, 78, [WLZ+12a]. 2pπ [VLFG12]. 3 [ABTW14, GWJ12, LQZZ12, LD17, RLW+13, SM14c]. 30 [GGD12, SLZ+12]. 3d [ALA15, DD17, RZC13]. 3dσ [VLFG12]. 4
[CD12, GWJ12]. \( m = 1 - 2 \) [FTB11]. \( m^* \) [Dw13]. \( \mu \) [ESS13]. \( N \)
[CZJZ12, CPL15, DDÇY12, DPRK12, DDF\+12, ES17, KC11, KSAK17,
MOSK10, MAN15, NIA\+12, Pan16, SFW12, CMCN11, CSK12, DFK16,
GE12b, KSSK16, KMM16, ZYZ\+11]. \( n + m \leq 5 \) [CD12]. \( N, N \) [dAVdM17].
\( n = [LHL\+15, SM14b], n = 0, 1, 2 \) [SKS10]. \( N = 1 \)
[SM16, CWSZ13, GGJD13, GB13, HDQ\+13, SR13, SM14d, WCS\+13, YC13,
BGMD15, PAKA15, SBB16, SM14c, BdjDMAV12, CD12, GWJ12]. \( n = 1, 2 \)
[BP\+10]. \( n = 1, 4 - 7 \) [FTB11]. \( n = 2 \)
[Ali14, HDQ\+13, MJ14, CDSK12, GGD12]. \( n = 2, 3, 4 \) [GP\+13b]. \( n = 20 \)
[SLZ\+12]. \( \nu \) [CZJZ12, DDÇY12, Tav11]. \( n \geq 2 \) [SM14c]. \( o \) [KSAK17]. \( p \)
[AGJ12, AMAC12, CSK12, DLJT14, HLZ\+14, RRK16, SRA\+11, ZSASS13,
ZYZ\+11]. \( \pi \) [BWE16, CC13, DWZZ15, KPL\+17, LDLB15, LB18, MC17,
MANP17, NMV\+14, PC16, SPD\+18, SSS15, TK16b, YZZ16, YD17, CC11b,
SLS\+12, AEGKZ12, BMR\+13, DB15, FV11, GNM\+12, LCB10, MMA10,
Nik11, NRGS11, RVPN12, RNV\+12, SD13a, VSS11, Yam10, ZZL\+11]. \( \Pi_n \)
[HHL\+12b]. \( \pi \cdots \pi \) [WLC\+117]. \( \pi \sigma^* \) [KG11]. \( \Gamma \) [Dau16, SAHA\+16]. \( \Psi^\sigma \)
[GS10]. \( q \) [Agb12]. \( q = 0 \) [SM14c]. \( \rightarrow \) [Buc12a, Coo12, LCB10,
MPPRCEG12, NWQQ11, YGL\+11, YZ10, ZH12]. \( \psi SU(2) \) [Brala]. \( S \) [HR12].
\( S = 1/2 \) [KLZQ15]. \( \sigma \)
[SPIL14, SC18, CC11b, Ang10, Che12, DCdG10, JLG\+12, Yam10]. \( \Sigma^- \)
[ZCG\+17, SLS\+12]. \( \Sigma^\sigma \) [ZCG\+17]. \( \sigma_{\text{hole}} \) [VVJ15]. \( \sigma \pi \) [XYY13, DMW11].
\( \sqrt{3} \times \sqrt{3} \) [OD16]. \( \times \) [PWL\+10, ZWWY10]. \( \rightarrow \) [KMM16]. \( v = 0, 1 \) [LZFZ13].
\( v = 0, j = 0 \) [YZ10]. \( \varphi \) [CC11b]. \( W(l, m, n; \alpha, \beta, \gamma) \) [IYW13]. \( \wedge \)
[ZQJW13, YLY\+12]. \( x = 0 \) [HCL13]. \( x = 1 \) [RLW\+13]. \( x = 2 \) [BCGC12].

* [LCB10].

-1 [CPL15, LL17, TAY11, YZW\+15a]. -1-methyl-1H-benzo [ÖEB11]. -2
[ZWWY10, JW12+12]. -2 [KDC12, KAOB11]. -2-ethoxy- benzamide
[FP12]. -3 [Tan12]. -3-methyl-cyclopentanone [PCR\+11].
-3-methyl-divinylene [FO10]. -4 [RS11b]. -4-phenylphenol [NVPC13].
[MANP17, KPL\+17]. -acetyl [Tav11]. -Al [MKF\+12]. -alanine [ZPR10].
-aminophenanthridine [VBO\+15]. -arylamides [DDF\+12].
-arylcarbamates [DDF\+12]. -azauracil [MPE15]. -based [MGP16].
-bidipyrrins [JW12+12]. -bis [SAHA16]. -bithiophene [SAHA16].
-bithiazoline [Qu13]. -bonded [SPIL14, DB15]. -Br [DVDBM11]. -butene
-catalyzed [LYR\+17]. -CF [LaY14]. -chain [EPS\+16]. -chloro-acetic
[DDÇY12]. -chloroaniline [HLZ\+14]. -chlorobenzaldehyde [SRA\+11].
-cluster [GP13b]. -conjugated [MMA10, GNM\+12]. -cyano-biphenyl
[RS11b]. -cyclic [Con10]. -cyclodextrin [NMHPVG12, SVRG12].
1H-imidazo [YB11]. 1I [GTR11].

2 [Boe12, EKD12, KK14a, LV12, Men10, MEEA+13, SAHAA16, Tan12, WWX+11, Zha14]. 2- [KOAB11, NVPCJ+13, OEDB11, YLW+13, Tan12].
2-adamantyl-thiazolidine-4-one [MBBT+12]. 2-amino [RJY+10].
2-amino-3-methylimidazo [MLPT10]. 2-azidoethanamines [SM10b].
2-carboxylic [KC11]. 2-chloroethyl [CZJZ12].
2-diazoo [LDW+11].
2-dichloromethylbenzimidazole [PMC11].
2-dihydro-3H-pyrazol-3-one [OPP+14].
2-dioxetanone [dSdS13b].
2-ethoxypyridine [MCC12].
2-furoic [GIO12].
2-hydroxy-3-methylbenzylidene [TAY11].
2-RDM [KK14a]. 2-substituted [Tug13]. 2.0 [CWW+16, LKZ+16, SC12b]. 3- [SC12b]. 3-alkylthiophene [BMR+13].
3-aminoacrylaldehyde [NRS+11]. 3-bisphospo-D-glyceric [SLA12].
3-imino-propenylamine [RJA+10]. 3-mesityl-3-methylcyclobutyl [KDC12].
3-methyl-1-pyridin-2-yl-5-pyrazole [PGG12].
3-Methyl-3-phenyl-cyclobutene [MB13].
3-Dimethylphenyl [Tan12].
3-dinitrophenyl [RNdA+10]. 4-diols [SBEH11]. 4-dioxane [Cha10]. 4-dithio-5-fluorouracil [NA12].
4-fluoro [YWJ+11]. 4-hydroxybutyloxy [RS11b]. 4-methylcyclohexylidene [KGVG11]. 4-phenylazoaniline [NVPCJ+13]. 4-triazol-3-one [CLY12].
4-triazole [LLW+11]. 4-triazolin-2 [IK14]. 4-trifluoromethylphenyl [SAHAA16]. 4-X-2-hydroxybenzaldehydes [EKN10]. 400K [KAR12a].
4965 [SKHN13].
Aluminum [ALK18, HTM10, IIW+11, Kar12b, MS14b, MM11, PMH+16]. Aluminum-bismuth-nitrogen [MS14b]. Aluminum-poor [ALK18].

[CWZ+10, DWZZ15, GXZ+14, HFL+17, LWZ+14, MTS15, ONBP11, Pat15, PM17, RGPD13, RGR12, YM12, YT14, ZLWL16, ZLWZ16]. anion-
[DWZZ15], anion-based [LWZ+14]. anionic [BMB12, GLPA10, XZL+12].
anions [Bar11, DZO12c, LCL+10b, MPM15, XSLF12]. anisol [AMAC12].
Anisotropic [BMTT11, LD2G16]. anisotropy [Ali14, MOY13]. annealing
[MOE+11, TCG17]. annealing-based [TCG17]. annelated [PPK+13].
anulation [ZQW+17]. anomaly [Kar12c]. ansatizes [Fin17]. Answers
[Tas14]. antihydrilic [MC11a]. anthropogenic [Mor11]. anti
[Iku17, MPE11, ScBsr+10, Zag11]. anti-Bragg [Zag11]. anti-Bredt [Iku17].
an-anti-inflammatory [MPE11, ScBsr+10]. antiaromatic [RBZ15].
antibiotics [LSR10b]. antibonding [CCL+16]. anticancer
[CZJZ12, MKHM11, PPK+13, XZ11]. Antidot [MY+13].
antiferromagnetism [Fuk12]. antiinflammatory [YIM13]. antigeniallary
[AB16b, LTtSJ+10, RDM+11]. antimicrobial [ESBVY12]. antioxidant
[KDA+11, KKLd1d, ZYL+13]. antioxidative [TIK11]. antiparallel
[SJW13]. antisense [UJS13]. antisymmetric [TKN13]. antitrpyconical
[MCL+11]. antityrpanosomal [LWH+12]. antitubercular
[SID1a]. antitumors [CCL+10]. antiviral [MB14]. any
[FMPP+14]. AP [NYS+10]. AP-UBD [NYS+10]. AP-UCC
[NYS+10]. apoptosis [QZH13]. applicability [BJ17, FCS13a, FCS13b, WKE17, ZT13]. Application
[ASK15, DSL15, ENV15, JH15, NMSR14, OVT+16, RZG12, Rom10, SCBP17,
TLC+17, TPCJ+12, Cha11, GFWZ11, HW12, KLK13, LLLT12, LVP12b,
MPD+15, MT10, dMOB12, SKV12, XWC10, AEM+12, DLRFMY10,
HBMN11, IKS08, IKS10, KPH12, Luz11b, LKd+16, MPReG12, MJ11,
PCR+11, RC11, SR12, SS12]. Applications [CW11, Lar11, MSNM18,
Nem14, SDF+16, AMAM18, CCl2, HKZZ15, Hll3, Kap12, LMZY15,
MANP17, MPMC+11, MML+16, MG12, MML11b, Nic11, SSS15, TSsL+16,
TSS+15, YKM+15, YFY17, ZSS14, CW13b, ZDZO10, Mor13]. applied
[BVRMO10, CF11, CL08, FCC11, HM11, NS13, SMV11, WR14a]. Approach
[LFF+10, ATL+14, AK17, AOB12, ART08, BPVB11, BvGW14, BV14,
BLKB11, CG18, DVDB11, DLM12, DMBL16, DLP17, Exn11, FAF12,
Frl12, FUE+12, GR10, GRD11, JLL11, KP10, KIt17, LBBW11, LSR10b,
LSR+13, LdaA+11, Mak15, MKG+11, MGN14, Msvmci10, MBB+12,
Mor12, NsNN17, NNpSN17, NvPcj+13, OT14, Opc17, OGvG18, P13, Pir13,
RZ17, RNC+14, RC11, RdPW+12, Sclcpb12, Saba+b2, Sba10a, SC12b,
Sps11a, Sbb12a, SD13b, Sc10a, SKL10, Toul11a, TPCJ+12, Uyn+b13,
WZ10a, WWb+b14, WR14a, XNL+14, Yam11, Yk13, dsdS13b]. approaches
[AMMK11, BBA+16, Cap16, CKL16, DC14b, EML+b11, IAK13, ILBS10,
Jia15, LMzy15, MDC15, Men15, NYS+10, PBB15, PJP08, Sko16, TS17].
approximate [FSB16]. approximants [DB13a]. Approximate
[HYZS12, ZLJ11, AST16, HMH10b, KY+b13b, Toul11a, ZRLV10].
approximately [KSN+b10]. Approximating [Fin16b]. approximation
[AY15, BC15, BC16, BR12b, Fin15, GZSMFN16, HM10a, IH16, Kut13,
Saba+b2, SK17a, Sut12, VV+b16]. approximations
[CLXD15, FMMD$^{+10}$, GZSMFN16, Per18, PBB15, RBD$^{+10}$, SGL$^{+16}$].


AROCM [ZPW16].

Aromatic [TKS11, BRS10, BG13, Bia15, CA17, KUTS10, KKS$^{+11}$, LVP12b, MLW10, MSL11, NHG$^{+12}$, PCML08, RVNP12, RBZ15, Ril10, SFM13, Sat11a, SM10b, TIKN11, MB14, MNE$^{+13}$, MPL$^{+11}$, PS10a, RZG12, RCM10, SM10b, TIKN11].


Assessment [LYR$^{+17}$]. associated [DL12, GI11a, MBTV12, WJ11, YKM$^{+15}$, dCSDdMC13]. association [NWQX11]. aspheric [For17b]. astrochemistry [For17a].

Atoms-in-molecules [OA13], attached [HMP\textsuperscript{11}], attachment [DSVP15, Kry12b], attack [LZFZ13], attenuated [NDP10], attenuating [CF14]. Attosecond [Vik11a, SVPTM\textsuperscript{10}], attractive [DCD11]. Au/SAPo [GSB10].

Au/SAPo-11 [GSB10]. AuCl [SM14b], augment [BDG17], augmented [CLKD15, D'y16, KRC\textsuperscript{+16}, SZS\textsuperscript{+10}, SLZ\textsuperscript{+11c}, SLZ\textsuperscript{+11a}]. AuO [SM14c]. 

Aureusidin [KK11d]. Aut [HYH\textsuperscript{10}], autocatalysis [Pic12].

Autocatalytic [dM13], autocorrelation [MPV\textsuperscript{11}], AutoDock [CRFR11], autoignition [MOH\textsuperscript{12}], autoionizing [Cor16], automated [MHO\textsuperscript{15}, PBB15]. Automatic [MML\textsuperscript{+16}, CW11]. AuX [LC16], auxiliary [CEFMK12, GS10]. averaged [ABLT11, CP13, RS12b, RSN12]. avian [KRH13, PCML08, WZ10a, ZBK15]. axial [LGS\textsuperscript{16}]. axiomatic [AK17].

axis [Lad14, XTLA13, XTLA14]. aza [DC14a, WWL\textsuperscript{11}, WLWT12].

aza-M"obius [WWL\textsuperscript{11}]. azanaphthoquinone [PPK\textsuperscript{13}]. azauracil [MPE15]. azide [Per10b]. azides [AEKGZ12]. azidoethanamines [SM10b].

aziridination [MCC13b]. azobenzenes [JPP\textsuperscript{11}]. azochromophores [FSB16]. azoc compound [NVPCJ\textsuperscript{13}]. azodicarboxylate [KI15]. azoles [SK12a]. azomethine [DI10, ZQW\textsuperscript{17}]. azoniaallene [WLWT12]. azopyrroles [Jac12]. azosulpha [EAK\textsuperscript{10b}].

B [BCGC12, CWS15, GWM11, JLL11, LCZ15, MLY\textsuperscript{+16}, PP14, VVAO12, WCS\textsuperscript{+13}, YGLL10, ADB10, CWSZ13, CD12, HWL16, HZS14, KGK13, LCL\textsuperscript{+10a}, SX5\textsuperscript{+12}, SCZG12, TCSD12, XLGA12, YGLL10, ZYL\textsuperscript{+14}]. B-like [SCZG12]. B-spline [HZS14]. B-type [XLGA12]. B/PR [GWM11]. B3LYP [JdOS16, Lu15, NDM\textsuperscript{+12}, WZ15b]. Ba [MPD\textsuperscript{15}]. BACE1 [VHTEG15]. 

back [LBdV16]. back-donation [LBdV16]. Backbiting [LSG\textsuperscript{14}].

backbone [PT13]. BaFe [WSCL11]. baicalein [MMM12]. balance [AZD\textsuperscript{+11}]. Balancing [TMC\textsuperscript{+13}, NMSR14]. band [BA13, CRSB12, DM16, IMS\textsuperscript{+13}, KA13, Lad14, SSB12a, VLM\textsuperscript{+10}, XTLA13, XTLA14, YHL\textsuperscript{+13}, ZQJC10]. Bandgap [WCL\textsuperscript{+17}]. bandgaps [GbZA10].

bands [BW15]. bandstructure [MMA10]. bang [CF11]. barium [MMR\textsuperscript{+10}]. barrier [CYK17, DLM12, DDF\textsuperscript{+12}, DCR10, LLF\textsuperscript{+12}, TCG17].

barrierless [dMOB12]. barriers [SCBP17]. Base [SM13, ACF\textsuperscript{+11}, AZD\textsuperscript{+11}, CPF12, CW16, EMSB15, KSS12, Kuv10, LSR\textsuperscript{+10a}, LSR\textsuperscript{+11}, Lad14, MSH13, OM13b, PP14, SMEH15, XSLF12, XTLA13, XTLA14, ZKWZ17, ZSQ\textsuperscript{+10}, dSTH17]. based [AB16a, ATM17, BP13, Bra10, Buc11b, BSO16, CWW12, CLC10, CwCW\textsuperscript{+11}, CLL\textsuperscript{+11}, CCG18, CL08, DIZ\textsuperscript{+10}, DTVP\textsuperscript{+12}, Dw13, DB13b, Exn11, FM16, 

[OA13, TBRIS12, AMK10, AM10, BSO11, Dil13, EMSB15, GBS17, GLT13, 

GZSMFN16, GI10, GI11b, GI11c, GI11e, GS11, Gra11, HMP\textsuperscript{+11}, IG11, 

JEA13, JMX\textsuperscript{+15}, Jol17, LKJ13, LZW\textsuperscript{+15}, LLH15, Luz11b, MOY13, 

MFLK10, MJ11, NS10b, NIT16, ONBP11, OD12, PRPU\textsuperscript{+13}, PWP13, 

RLW\textsuperscript{+13}, RD14, SBMM11, SBM16, Sto18, SKL10, TBRIS10, TBRIS11, 

TH12, TLC\textsuperscript{+17}, YJ17, ZSI11, ZCG\textsuperscript{+16}, ZHI17, ZJS13, dSTH17, dCGAMV12].
FT15, FKC12, FSST16, GZ14, GZMC11, HJK14, HW12, JMX+15, Jeo18, JNZ+14, KKM+12, KSAK17, KYH+13b, Kry12c, LPO+12, LCL+10a, LV12, LQZZ12, LXW+14, LCK+16, LXD13, LLZ+14, LWZ+14, LEU+11, Mag14, MDC15, MANP17, MCP10, MGP16, NKF+13, NZ13, OPS10, OAT+13, PI13, PABSK16, Pir13, PSM11, PMAP12, PSK+13, RS11b, SYK+12, SKHN13, ST15, SK11, SLZ+12, SSS15, TCG17, TMC+13, TK16b, Tsu15, WKE17, WJY15, WYM15, YZ13, YZZH15, YKN13, YSW11, ZKW17].

bases
[BS14, EG10, EAV16, GGP13, MMR+10, PS10a, XZ11, Yak11, YDW13].

basic [GI11b, GI11c, BM16, KK14a, Nic11].
basicities [VF13a].

basics
[HFL+17, SM16].

Basics [Bae16, Mos14].

basins
[HS11c].

Basis
[JA12, KY13].

batteries
[KLK13].

battery
[KJ15, Oni12].

BAu
[LL11].

Baylis
[ZQW+17].

BaZrO
[GMP+11].

Basics
[BA11, B L16, BVCAP12, CML+16, DCZ17, Fuk12, GTR11, Hil13, Hog13, JH15, KRC+16, KUY16, Knt13, Lai11, LV12, LWL+12, MSNP18, MG12, NDM+12, PC14, RLER14, RVO+14, RLZ12, SKTI15, SZS+10, SLZ+11c, SSL+11, TCG17, TWR15, UV18, VSS11, WS10, YMY15, YZ13, YZZH15, YKN13, YSW11, ZKW17].

bath
[YK13].

batteries
[KLK13].

battery
[KJ15, Oni12].

BAu
[LL11].

Bean
[BMB12].

bearing
[CMR13, MCK17].

BEC
[GdLT12].

Behavior
[GST11, DSC+11, DLM+11, LG12, RF10, RGS+13, SHE10, SM14c, SMGZ13].

behaviors
[HKLW13, VSL+15].

Benchmark
[JZZH17, PB10, HM12, LP10b, OKR12, RS12a, RS12b, RS12n, Vie17, WZW17, YWH12a, YWH12b].

benchmark-quality
[OKR12].

Benchmarking
[KDOR17, Man16, MBSAG16a, PRFR17, MBSAG16b, Rus14, VBJK18].

benchmarks
[Lat13, LJ13].

bending
[GFB12a, IMS+13, ZZ15].

bent
[HV11].

Benveniste
[WSV10].

benzal
[YWJ+11].

benzaldehyde
[ZSHL14].

benzamide
[DPRK12].

Benzene
[CGM12, CL11, CCS13, DKZ+10, DJ18, FZH+18, HqGZ17, KBBM10, SPSA11, Sch12a, TG13, VC13, WDSL14, Yu13, ZS12].

benzenoids
[BR08, BR12a, RB08, RB11a, RVNP12].

benzimidazole
[WLL+13].

benzimidazoles
[LZB10, XFW+14].

benzimidazolyl
[SHW+13].

benzo [ÖEDB11].

benzoazacrown
[FBU+11].

benzoazacrown-containing
[FBU+11].

benzocatafusenes
[MA12].

benzofuran
[ASMP15].

benzoic
[SN12, SHL+13].

benzoic acid
[ZSHL14].

Benzothiadiazoles
[Net12].

benzoic acid
[YLW+13].

benzonitrile
[LD17].

benzylic
[EHKD11, EKD12, SJZ12].

benzylic acid
[DCY12].

BeO
[Nic14].

BEPOX
[KZZ13b].

Berry
[DAB12].

Beryllium
[BN12, DZO12b, Nic11].

BeS
[DAR+11].

Best
[Ish14, CB10].

beta
[MBTVR12, PTD+12].

better
[BL+13].

between
[ASHF13, AD17, BLR12, BL11, BLWJ17, BWE16, BB16, CZZ12, CCL+13, Cha10, CCS13, CF17, DNCKCS+12, EKN10, EHKD11, EKD12, EEMSS14, EAV16, FIN16a, FIN17, GXZ+14, Gra08, Gra11, GE12a, HMM+13, JEA13,

Bound-states [Agbi2]. Boundary [LZ12, CW13b, MFLK11, UYN+13].


C [Ban12, BCP10, BGFD14, DQZF12, GWM11, GZW16, GB13, GCD13, JLL+18, JLG+12, KI12, KN15, LKN13, LCS+11a, MLY+16, MGD11, NBL12, OGSg18, PAK15, PP14, SU+11, USL+13, VF13a, VLK+11, WLZ+12a, WLZ+12b, WZV17, WSL+11, YK11, YZL+10, YLZ+17, YL11, ZQJW13, ZW15, ZLWZ16, TSNK12, YB11, CCEGK12, CWL+13, CRSB12, CTDOLA10, DFK16, DSFT17, EML+11, FBRBR12, FBO+11, GB13, HV11, HHL+12b, IMS+13, JCCZ12, KWC10, KZA+17, Kan11, KK11b, KK12a, KL12, LCL+10a, LBY+14, LZW+15, LCZ15, LXD13, LW15, LdAA+11, MNV+17, MSS11, MIN13, MS17, NL11, NMIP14, Nik11, Pts+11, PAK15, R11, RR21, RCO11, SBAT16, Sat11b, SHTW10, SW12, SYZ17, SC18, TG13, TK17, WCSS+13, WZGW17, XCY15, ZPM10, ZLWL16, ZJC+13, DZO12b].

[PAKA15]. cages [NW12]. calcite [SC11]. calcium [Ish14, RCGLV+14].
calcium-doped [RCGLV+14]. calculate [ZLE17]. Calculated
[SPO+11, Dw13, FKL+12, MFK+12, VMC11, WWC17]. Calculating
[FYhC11, KC11, WB17, ARH+13, CML+16, MGK+11, SA11a].
Calculation [FZC14, KKS+11, MHO+15, Rit12a, SHS+13, VLFG12, VO11, YSÖ12, AM12,
BVCAP12, Boe12, CP10, DK13, FLCHL10, FBM+10, FSB16, GWZ+14a,
GCDNGS12, HMI+15, IK18, KMK+16, KHH10, Kri13, LIK15, MGK+12,
Man13, MA12, Mit11c, dMOB12, PS10a, Per10b, PCR+11, Rit12b, SBM16,
ST15, SRASZ16, TTT13, VF13a, WZH13, YK13, YM14, YH14b, YLYC18].
calculateal [SC12a]. Calculations [KH10, KV11, LKJ13, TWHZ14,
dHLs12, AK17, AFA13, ADB10, ACMRN10, Bas11, BB10, Bou12b, BJ12,
Buc11b, Bud12, COCF+14, CK17, CSTA16, ČFČ11, Dan16, DSL15, DAE+12,
DWX+16, DZO12c, DZO12a, DFF+13, ESS13, ENG16, FSK+11, GVPCK10,
GSaY11, GZF13, Glu13, GE12b, HK11, HHCA10, HS11b, HZH14, JH13,
KAR12a, KK14a, KG17, KRK+17, KSS12, Kim13, KJ15, KJ16a, KJ16b,
Kin13, KYH+13b, KPH+12, KKG12, LRP+11, LCL+10a, LC16, LCK+16,
LLZ+12, LNI12, MJ16a, MVC13, Mit11b, Mit11a, MPL12, MSY+12,
MPT11, MPTZ13, NMSR14, NZLG15, yOITn15, OKK10, OPP+14, OSJ+12,
PK16, PB10, RS12a, RZG12, RLER14, RAMB18, RCGLV+14, RVO+14,
Rud12, RRCO11, RTT10, RMY+13, SMEH15, SAHG11, SAHA12, SL13,
Sko16, STL12, SRA+11, SN11, SW12, SJW13, SCBP17, Tan13, TNN16].
calculations [TSH17, TWR15, UTtn13, USL+13, VVBB10, Wagy14,
WWC17, WYM15, WZW17, YYI+12, YYY+13, YSK+12, YKM+15, YHL+13,
Zak13, ZST+10, QJCJ10, ZCC11, ZF15, ZZZ12]. CAM [JdOS16]. CaMn
[SYK+12, YYY+13, YYY+13, YSK+12]. Can
[Lu15, Met11, Nes11, Sza13, TFA10, BSo15, Luz11a, ZLWL16]. cancer
[LB14a]. candidate [AB16b]. candidates [KMRG13].
Canonical [GW13, CCL+16, JH15, Jor15]. Canuto [Ano11a, RdA11]. CaO [SAHA12].
capules [KKH+13]. capture [GaSY11, Mai14, PRP+13]. carbasol
[MUnZVR12]. carbazol-oxadiazole [MUnZVR12]. carbazole [ZBBB17].
carbene
[LWC+10, LCS+11a, LCH+11, LCS+11b, LXLL11, RMP+14, ZFS+11].
carbenes [ABTW14, MAN15, Pan16, SZL+14]. carbide [NEEV15, RK14].
carbides [GM11]. carbocyanine [Mas10]. carboxydiimides [WLWT12].
carbodithioic [SJZL12]. carbonylhydrazide [HZZW11]. Carbon
[DSFT17, MPL+11, AKC10, AEM+12, Bas11, BEPZ10a, Buc10, Buc11b,
BSO11, CS13, CTDOLA10, DI10, DM16, EBR11, GAMM10, GT13, GP13,
HNBG15, Hog13, KKC14, KKT13, KKT14, KG08, Mai14, MOSV13, OPS10,
OD12, PP14, RKK16, SD13a, SC10a, SQ10, TDOD17, TC10, Wan11, WW11,
WHY+14, WJY15, WDJ+17, Yam10, ZCX+16, ZMB+17]. carbonate
[DL016, YM12]. Carbonates [RBLZ15, ZQW+17]. carbonic [dM13].
carbonmonoxy [CHSO13]. carbonyl
[BH10a, DWJZ11, GGJD13, MTS15, MG10, YYS15, dCSDdMC13].
carbonyl-coordination [GGJD13]. carbonyls [LLW+12]. carborane [FSQ+11, LCZ15]. carboxylates [HhGqZZ17]. carboxaldehyde [TBA13].
carboxylase [WLD+10]. Carboxylate [SCB+14, KSAK17, LYL+12].
carboxylic [KC11, LGM+18, MK10b, SAG13, TPT+13, VF13a, WJ11].
carcinogenic [DKZ+10]. Carlo [ÁFV12, ABG12, ANC+15, ASK15, Cal10, CP16, Hog13, HB14, HM12, JCCZ12, PDR+14, RCGLV+14, SGC13, SCBP17, Wag14, WCM14, ZLR15, ZCC11]. Carlos [HS15].
carrier [GNM+12]. carriers [NMV+14]. cascade [Fra17].
case [AGRI+12, BDF+16, Bas11, BBM17, CCL+16, DMAB12, DVDBM11, DAA16, DCDD10, DFF+13, GS11, Mar12, MVG18, MSC10, MURR13, Oni10, Ped16, PK13b, SS10, TC12, TWR15, YLZ+17, CTVA12, DB12].
cases [Zak13].
CASPT2 [BDFM10, BDR12, ČFČ11, GLOGM+11, KZZ13a, LCL+11, LGP+12, MR11, Pul11, RS12b, SKTI15, SGC13, SCBP17, Wag14, WCM14, ZLR15, ZCC11].
CASPT2//CASSCF [GLOGM+11]. CASSCF [BDFM10, DAR+11, GLOGM+11, Lar11, Ols11a, PE11, RS12b, RSN12, SZZ+12, SBL11].
CASSCF/CASPT2 [SZZ+12, BDFM10]. CASSCF/MRCI [SZZ+12, BDFM10].
CASSCF [BDFM10, DAR+11, GLOGM+11, Lar11, Ols11a, PE11, RS12b, RSN12, SZZ+12, SBL11].
Catalyzed [AKC10, AZD+11, CWZ+10, Che12, GCZ+14, JL12b, JSLH14, KUTS10, LGM+18, LZZ12, LQ13, LYR+17, LLF17, LD17, LMCZ11, LCZL11, LW13, LW15, LKZ+16, MCC13b, PRFR17, SHL+13, SR11a, SLS+15, TTD13, TFA10, WML10, WWL17, WWZL10, ZCZ+12, ZSHL14, ZZZ15, ZQW+17, ZSS+13, ZLY+14, ZPW16].
catechin [MKHM11].
catecholamines [MBTVR12].
cation [ZLWZ16, ATS+11, Ber13a, DWJZ11, DAE+12, HV11, LCL+10a, LLC+11, MMM12, MS14c, ONBP11, Oni10, PDR+14, PvS10, SPSA11, SZZ+12, XZL+12, YM12, ZFC12].
cavity [Pup11a].
cavity [Pup11a]. Cavities [Pup11a].
ce [SLS+11]. cc-pV5Z [SLS+11].
cells [AGJ12, BDG17, FFPD16, FM16, cLqFtW+14, MY17, PMAP12, TZ11, ZSAP11, Zha17].
cellular
cis- [FMKJ14, KZZ13b]. cis-7 [LCB10]. cis-9 [LCB10]. cis-trans [BSM+15]. Cl [DS12, EMSB15, EMS16, FBO+11, GB13, HJRO13, HNBG15, JLG+12, LMZ+11, LLG+12, LWL+12, LSS+11a, MZL17, MEEA+13, MPRCEG12, SBS10, SD12, SPI14, SYQ+10, SZL+14, TL15, WZW17, XZL+12, DZO11, KZA+17, LLLB13, LdAA+11, Ma14, OKR12, SM14b, SC18, XZYS10, YGL+11].


ESS13, EMSB15, EMS16, FBRBR12, For12, FBD+13, HS11b, HYD11, HZZW11, KRK+17, KV11, Kry12c, KBMM10, LJL+11, LYW11, LXW+14, LYR+17, LYL+12, LXD13, Lu10, MZB+13, MCE11, MNV+17, MC17, MC12, Men10, MG12, MKM11, MS14c, MPRCEG12, ND11, NDF+10, OAC17, OPP+14, OVT+16, Owe17, PCMG12, PRG+10, PAKA12, RFEGPP+16, RB11b, SS10, SVRGV12, SGKG12, SRASZ16, SAHA12, SLS+14, SK11, SSP+17b, SPL14, SHW+13, SM17, SK12b, SS13, TTD13, TMM+14, TL15, UDVI10, VO12, WX8+11, WZW17, WHM14, Wu11, YZL+10, YZL+11, YZW+15a, YWH+12c, YZZ16, ZPR10, ZLMS10, ZQ1V13, ZLZ+14, ZSC15, ZSQ+10, ZFS+11, ZLW16, ZSZ14, ZQ1P17, ZBBB17. complexity [EMED+12, SMOD11]. component [CW16, FZC14, KKT13, KKT14, MHT+08, SN15]. components [LVP12a, Nal12, RLZ12]. composed [TK16a]. Composite [KO10, ZJS13, Mor12]. Composites [KT12b]. composition [GLF+12, GbZA10, IBA+11, Ld11, LKN13, QZH13, XTLA13, XTLA14]. composition-dependent [LKN13]. Compound [ZST+10, KWC10, LLLB13, MQA17, PGG12, SKS10, SSW16, TYL10, TXL10, WR14b, vL13]. compounds [AMK10, BG13, BHI10a, Buc11b, CCA+12, CHV14, GZM11, HZG12, KMI2b, LOHB13, Ld10, LWJ10, MLC+11, MPDMC+11, MW16, Mor12, MSRN+11, PI13, PH12, Pie11, RDM+11, RRK16, SMC18, Sh13, TSv+16, TWR15, VPGC12, WCY+10, WWQG17, Y1W12, ZFC+17]. Comprehensive [LKN13, RYM12, WJY15, FK12, KI15, SL10]. compressed [Man16, MBSAG16a, MBSAG16b, SBM16]. Compton [Kar12c, Kar15]. Computation [CW13a, Sic16, YC011, ILB10, Kar12b, KY13, KZ13a, RBD+10, WKE17, Zen11, GI11c]. Computational [AM13a, AMK10, BYAT13, BJ17, BBA+16, BCS+12, CSM12, CT14, EM17, EBH11, FFP16, For17a, FNT16, GGJD13, HNBG15, Hor13, HCL13, IMS+13, KTH13, KYS13, KyH13a, KB17, KYH+13b, KFS13, KG13, LKOS17, LPOP12, LFS+11, LSR+13, LC10, LC11, MSG16, MK12, MANP17, MMF+13, NMF+13, Nym14, OAC17, OH13, OM13b, PS13a, PRG+10, PAPCM+16, PSK+13, PPK+13, RW11, SBAT16, SK14, SB10a, SKHN13, She12, She13, Sh13, SR11a, TYN13, TV13, THSR13, VSM15, WXZ+11, XTLA13, XZYS10, XZCH11, Y1Y+13, Y1Y+13, YMY+13, ZK12, ZQJW13, ATPRV11, ASU+17, AKC10, ASW13, Bar16, BDG17, BB16, CLXZ12, CPCS16, DLO16, DGA+13, EA12, GW11, GLPA10, HFL+17, JK12, KDC12, Kry10, LFF+12, LB1V6, MK10b, MEF+15, MM11, NBZG16, Nm14, PDNC14, Ped16, SGB11, SDP+16, Ser11a, SJ1Z12]. computational [SMA11, TAY11, Tan12, Tch13, TT10, TU10, WML10, WLL+13, YBMK12, ZSC15, Zha15, Zyl+13, ZCG+16, ZBBB17, ELC08, JLL+18]. Computations [GLT13, IA13, KBF+13, KKH+13, KKT13, LLM13, MOY13, McC13a, MNE+13, ONK+13, OA13, TIN13, TM13, BBB+12a, PI11, PB10, RS14, TTC16, Yu13]. compute [SGH10]. Computed [SUL+11].
corrosion-inhibition [THSR13]. cosine [GH11, GE12b, LLH15]. Coulomb [SS12, CF14, ARG11, BPL13, BBL12, Fin16b, FRGC10, Fuk12, GH11, JH13, KH12, KWWH18, KK13, LLH15, Luz12, Nag16b, NDP10, PGGRMP10, Rit12b, Roy13, Roy16, SMOD11, Sil14, TC12, ZX12]. Coulomb-attenuated [NDP10]. coulomb-attenuating [CF14]. Coulomb-like [PGGRMP10]. Coulombic [Roy15, YW11b]. Coulombic-like [YW11b]. coumarin [MDNDO+16]. Counter [XLGA12, ZLWL16, Oni10]. Counter-ion [XLGA12]. counterpart [KC16]. counterpoise [KPH+12]. counting [JL12a]. Coupled [BJ12, Cam10, Cam12, Sto18, VVVB10, WWC17, BVP13, BVP14, BSM+15, CSVCB12, DMAB12, DLM12, LRP+11, LP10b, Luz08, MPT11, PB10, RS12b, RSN12, SZA+10, Sza13, Var11, XDM+10, YK13]. Coupled-cluster [Cam10, Cam12, LP10b, PB10, SZA+10, Sza13]. coupling [ATL+14, BJ12, BSV12, CFGC11, CSP+10, CDT12, IROW10, Kry10, Lar10, LKOS17, LW15, MC18, PM12, RCP14, SSI+10, SHS+13, YSS+10, YH14b]. couplings [HKLW13, Kaw15]. course [HSYM11]. covalency [MML11b]. covalent [ABS13, AB16a, MURR13, NE11, KK13]. covariant [Luz08]. 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, Ano14a, Ano14b, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n]. Cover [Ano14p, Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n]. COX [MPE11]. COX-2 [MPE11]. COXIB [OSJ+12]. Cr

D [IS+17, Kan11, STL12, SYZ17, TSL11, XLLZ10, ZGSM15, CC11a, ÖEDB11, BEM12, DLRMFY10, HGB08, KH10, LCL+10a, LQZZ12, LLZaH14, NF11, OD12, PDT+12, QTCL10, SLA12, SSS15, SK10, WTH+11, YGLL10, YSW11, ZH12, Cys11]. D- [SSS15]. D-dimensional [DLRMYF10]. D-wave [KH10]. DABA [Ser11a]. DABCO [LLF17, LD17]. DABCO- [LL17]. DABCO-catalyzed [LD17]. damage [FMP+17, POLV12].


Density

[ALRA10, ALRAE11, BPL13, Fin15, LS17, MT11, WGLX10, ZL12]. Density
[Alw13-49, BGBV12, BjdMAV12, CCL†+13, CM12, CD12, DCCB11, DQZF12, EM16, ED16, FZX18, GGD12, HLZ†+14, HKLW13, HYD11, ISN13, IKN13, JS17, Kar13, KCC13, KK14b, KSRAK17, Kit14, Kit17, Lae14, LWL†+12, LWX†+14, LBY†+14, MLC†+11, MW16, MUNZVR12, MIN13, MLB†+12, MM13, MCRS16, MOH†+12, NTNL10, NZAVR10, PS10b, PS14, PMH†+16, RGPZD13, SVRGV12, SKY†+13, SS13, TOSN12, Tan12, TIN13, TDOD17, TFZ†+15, UMS13, VUC13, WJL†+11, YKM†+15, YL11, ZCX†+16, ZRR†+11, dCSDDMC13, ABLT11, AM13b, ATM17, AGPDZ13, AST16, BMK†+14, BD14, BCGC12, BDF†+16, BLKB11, CDSK12, CEFMK12, CM15, CNSK11, CH17, CZLD17, CLH14, CK17, CF14, CC11b, CSTA16, DWJZ11, DKS11, DPRK12, DW12, Dii13, DZ11a, DGR†+16, FO10, FDNR10, Fin16a, Fin17, FA17, FSB16, GCK†+17, GM11, GHCMCMQ17].

density

[GD11, GCZ†+14, HHCA10, HMH10b, HHIKH13, HZZW11, IN15, JR12, JPP†+11, Jan13, JW18, Jeol18, Jou13, KK13, KJ16a, KJ16b, KKL†+16, Kit15, KDD017, KJ14, Kri13, KFS13, KG08, KMU†+13, Lat13, LPO†+12, LSR10b, LWL11, LC16, LSP†+16, LLW†+11, LCK†+16, LDZ16, LNI12, MYZ†+10, MLW†+14, MJ16a, MFK12, MNS11, MJ11, MBBT12, MCRS16, MUNZVR12, MIN13, MLB†+12, MM13, MCRS16, MOH†+12, NTNL10, NZAVR10, PS10b, PS14, PMH†+16, RGPZD13, SVRGV12, SKY†+13, SS13, TOSN12, Tan12, TIN13, TDOD17, TFZ†+15, UMS13, VUC13, WJL†+11, YKM†+15, YL11, ZCX†+16, ZRR†+11, dCSDDMC13, ABLT11, AM13b, ATM17, AGPDZ13, AST16, BMK†+14, BD14, BCGC12, BDF†+16, BLKB11, CDSK12, CEFMK12, CM15, CNSK11, CH17, CZLD17, CLH14, CK17, CF14, CC11b, CSTA16, DWJZ11, DKS11, DPRK12, DW12, Dii13, DZ11a, DGR†+16, FO10, FDNR10, Fin16a, Fin17, FA17, FSB16, GCK†+17, GM11, GHCMCMQ17].

density [VSL†+15, WKE17, WW11, WJY15, WDJ†+17, WTB†+11, WR15, XNL†+14, XSLF12, XGR†+18, YWH12a, YWH12b, YRN†+11, Yu13, YF16, ZT13, ZKKR11, ZQJCJ10, ZLW13, ZMZ13, ZCG†+16, ZSIZ14, ZK11, dCGAMV12, CTDO1A0, LLZ†+12, Ven12]. Density-based [ZW17].

density-dependent [IN15]. Density-functional

[ZF18, BDF†+16, BLKB11, CF14, DW12, JR12, LNI12, MYZ†+10, WR15]. Density-functional-theory [SVRGV12]. Density-matrix

deoxiribonucleoside [MB14]. Dependence

[AG10a, BLWJ17, BUC12a, BN11, BS12, CAAN12, GLF†+12, KP11, KSG†+12, KKH†+13, LZZ13, Mar11, MIN13, MKS13, PMMGL†+11, Rud12, WR15].
dependent [Bae16, Bae14, BDF†+16, CP10, CEFMK12, CW11, CW13b, DCZ17, DM16, FMMD†+10, GSR12, HS11a, HHA10, HKZ115, IN15, ILBS10, IG11, JPP†+11, LKN13, LMZY15, Luz13, NMS†+10, NNS17, NNSN17, NDP10, Oht13, PVS12, PVS12, PSC15, PJP10, PMAP12, PI16, SFC16, SSAM13, SL13, Sko16, SHW†+13, Vik11a, Vik11b, WKE17, WYWL13, YLYC18, ZQJCJ10, ZCG†+17, ZLE17, ZS14]. dephasing [Gan14].

Depicting [LBdV16]. depolarization [AEM†+12]. deposited

[SAHG11, SAHA12]. deposition [TFBG14]. deprotonation
TG13, Tug13, TKSK17, UV18, VF13a, VLG12, VSN+11, Vie17, WLWT12, XX12, XZ11, YYS15, YY18, YY1+12, YIL1+13, YWY+12, YZW+15a, YZZ16, ZSAP11, ZLWL16, ZL10, ZQXP17, ZLY+14, ZPW16, ZCP11, ZDZL11, dSdS13a, dSdS13b. DFT-based [BP13, Dw13, MCP10].


DFT/TDDFT [Vie17], dG [XLGA12]. di-enol [Val17]. di-lanthanide [OAC17].

Diagonalization [CHM+17, ART08, DMAB12, DM12, KUY16, SHS+13]. diacetyl [TM13].

diatomic [Agb12, BKM15, BB10, CP13, CJOOW11, GM11, GS11, HRT12, Ish14, JZP17, KBGC12, KBG17, LLP17, MPM15, NDH10, RC11, Roy14, SY16, Ton11a].


dibenzothiophene-like [VPGC12]. dibenzothiophene [VPGC12]. diborane [ZYL+14]. dications [Buc12b, GN+12].

dichloro [LS+11a]. dichloro-germylene [ZYL+14].

dichloromethylbenzimidazole [PMC11].

dichloropropene [ASMP15]. dichlorosilylene [LLLB13].

dichoisy [PCR+11]. diabolic [Agb12, BB10, BP13, CJW11, GM11, GS11, HRT12, Ish14, ZLWL16, ZLY1+14].

dielectric [CN12, KPT12b, Ng12, NDM+12, OA13, Ser11a, Ser11b].

diels [CM12, Iku17, LW11, ZLWL16, ZXY13].

dienes [CW16]. dienone [KAOB11].

diethyl [KI15].

diethylcyclobutanones [Dum12].

diffusion [Wi12].

diesters [Buc12b, GN+12].

difluorohydroxyborane [MMCN+11].

dihydro [LLB13].

dihydrouridylopyrrolopyrrole-thiophene [MSG16].

dihydrobenzimidazole [KKG12].

dihydrobromide [SG12].

dihydrochloroamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].

dihydrodicyclohexylamine [SG12].
**Dimensional** [DTF⁺11, ART08, Beh15, BEPZ10b, Cho15, CYK17, Dau16, DLRMFY10, Dw13, DMS⁺10, Mam13, MPD⁺15, MDC15, MSC10, MLDP10, PGMRM15, RNC⁺14, SPD⁺18, SD13b, SSAM13, VBC⁺12a, VBC⁺12b].

dimensionally [Yam11]. dimensions [IIH16, RPVM10, RAK10]. dimer [AM13a, BF11, GIO12, HM12, MPT10, NVI10, NHB12, PMMG15⁺11, SKY⁺13, SS13, TNN16, Zak13]. dimeric [Rua10].
dimerization [LSR10b, Rua10, SKTI15, TFA10]. Dimers [TBRIS12, BCF⁺11, Cas15, FSB16, KM12a, KK11a, KDOR17, MT10, PP10, RPBB11, RNE10, TBRIS10, TBRIS11, TPT⁺13, VSS11, WJ11, dSCC12].
dimetal [ZFC⁺17]. dimetallic [LYD⁺18]. dimethoxyphenol [Tan12].
dimethyl [JSLH14, JAB12, LdBF⁺12, LXLL11, NMHPVG12, Owe17, SJZL12, SSP14, SCZH16, TAY11, TXL10, WXZ⁺11].
dimethyl-germylidene [TXL10]. dimethyl-silylene [LXLL11].
dimethylallene [CPL15]. dimethylamine [LLZZ10].
dimethylaminophenyl [FO10]. dimethylaminopropanol [WZX11].
dimethylcyclobutene [MB13]. dimethylmethylene [LWC⁺10].
dimethylnitrosamine [LVdSdM14, dAVdM17]. Dimethylphenyl [Tan12].
dinitrophenol [LDW⁺11]. dinitrophenyl [RNdA⁺10].
dinitrosamine [JN13].
dioxidane [Cha10, CNSK11]. dioxetanone [dSdS13b].
dioxide [JLS13, KKT13, KKT14, MPL⁺11, PP14, TDOD17].
dioxin [MSY⁺12].
dioxy [KMK⁺16]. Dioxygen [MMA13].
diphenylformazans [TT10]. diphenyl] [YWJ⁺11]. diphenylamino [CRSB12].
diphenyl-polyenes [MMWA11].
diphenylnitrosamine [VSDdM14]. diphenyl] [GAVdM17].
Dimethylether [Tan12].
Dimethylaniline [LLZZ10].
dimethylnitrosamine [LVdSdM14, dAVdM17].
Dimethylphenyl [Tan12].
diproton [EDA⁺16]. dipolar [BL11, DI10, ELC08]. dipole [AM12, Ber13a, Ber13c, BVP14, GFB12b, GI11a, GI11c, HK11, IMS⁺13, KA11, LKJ13, MA11b, MD11, MNS11, SS12].
dipoles [SMEH15].
disarm [NP18].
discontinuously [GB10].
discotic [SSKS12, ZSASS13].
Discrete [DTFK15, JCC10, TIKL13].
disease [Bal16, MPTR12].
diselenide [Dim12].
diselenide-linked [Dim12].
dismutase [CWZ⁺10, PM17].
disorder [PDR⁺14, Wan13].
dispersing [ISRK12].
Dissonance [KH12, Dob14, ISN13, IN15, KDO17, LCT14, MS17, PSC15, Pit12, SKY⁺13, WJY15, dCD⁺11].
dispersion-corrected [MS17].
dispersion-improved [LCT14].
dissipative [PD11].
dissociated [MT12].
Dissociation [CK17, GM11, PW10, SSW16, SM10b, BMBD10.
Bla15, CC11b, GSaY11, GLT13, GD11, KWC10, KZA+17, KTI+12, KMM16, LLL16, MMBK12, MNE+13, OK16, dMOB12, OKR12, RPBB11, Rua10, SLZ+12b, SB10a, SQ10, SYS14, SDY16, SCS15, TJS17, VSMK13, VO11, XX12, ZZX10, ZCC11, ZSHL14, ZZZ12, dSNBGO8. dissociations [TCA10].
dissociative [LCB15, Kry12b]. dissolution [KLK13]. distance [GI11b].
distortion [CL11, YY1+13]. distortions [GBF12a, GHCMCMQ17, PK13b].
distributed [RAMB18]. distribution [ABP13, DPRK12, EPS+16, GGD12, LGHL11, PK13a, RCM10, SM14a, TMM+14, WZX11, vLRRK15].
distributions [LBZV16, SVPTM+10]. distyrlypyridine [MUPC10].
disubstituted [dOdONM12, dSNBGO8]. disulfide
[Jan10, KKT13, KKT14, WXZ+11, WHY+14, ZMB+17]. disulfides
[GSaY11]. dithio [NA12, PS13a]. dithio-substituted [PS13a].
dithiolene [SRD+13, ZLW16], 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 [dILIA12]. divinylene [FO10]. DJ [Shi13]. DJ-1 [Shi13].
DMABN [CFP+10]. DMABN-Crown4 [CFP+10]. DMABN-Crown5 [CFP+10].
DMAP [LLF17]. DMAP-catalyzed [LLF17]. DMC [Ryw+15].
DMRG [MFLP12]. DMSO [VLk+11, CCL+10, SK12a, Ven12, YZZ15].
dmso-S [CCL+10]. DNA [Lad14, XTLA14, ACF+11, BS14, BBM17, CLC10, CW16, Che13, Coo12, DTFK15, DSVP15, EG10, FV11, GilWZ11, HW12, KZA+17, KK5+11, LCH14, LQZZ12, LLZ+14, MMR+10, MS10, Net12, OM13b, POLV12, PAD+10, PPK+13, RAK10, SM13, Sza13, XLGA12, XTLA13, Yak10, Yak11, ZM13, ZTC11]. DNA-based [LLZ+14]. DNA-bases
[EG10]. DNA-binding [BBM17]. DNA/RNA [BS14, KZA+17]. DNT
[LPO12]. do [HST13]. Docking
[LDMDCA+12, Net12, CSVCB12, CSSK+12, RdPW+12, WYY+12]. DOD
[FY17]. DOD-PBEPP86-NL [FY17]. dodecaborate [LYR+17].
dodecyl [CAPL12]. Does [BN12, BuR12, Fin14b]. Domain
[ABL11, CP13, Pat15, ZLE17]. Domain-averaged [ABL11, CP13].
domain-restricted [ABL11]. donation [DCdG10, LBdV16]. donor
[ABA11, BLL+13, CMR13, IIS+17, KPL+17, LQ13, LGS+16, MANP17, SSK11, ScB5R+10, TSBSM12, ZKKR11, ZFS+11].
donor-[MANP17, KPL+17]. donor-acceptor [ABA11].
donor-peptide [SSK11]. donors [CN12, VVJ15, WTW+15, XZYS10].
dopant [RMTG11]. dopants
[VSMK13]. Doped [XZM+12, ASW13, BSS15, CSK12, CWW+16, DVBMM11, DWX+16, ENV15, FFPD16, FTB11, Gamm10, HLMO11, HNBG15, HWL16, KJ14, LHL+15, NW12, Oni10, OGvSG18, RKM12, RZC13, RYW+15, RCGLV+14, SD16a, ZCX+16].
doped-gold [FTB11].
doping [BGL+16, Fer11, OH13, PPDF11, TW10, YY1+13, ZK12]. dot
[CSK12, CN12, LEU+11, MR12, RP11a, YH14a, ZX12]. dots
Double [CF14, SLZ+12, AF16, CF17, KKC14, KMT+12, LV12, NBL+14, PAD+10, PM17, SDL+15, VAT12, WZX+15a, Xu16, Yu13, YF16, ZX12].
double-excitations [VAT12]. double-hybrid [AF16, Yu13, YF16].
double-well [SDL+15]. doubles [HFD11]. doubly [BMF13, Cor16, KT12a, SX15].
Douglas [SN15]. down [RF10].
doxorubicin [Bas11]. Dr. [Mer11]. Dressed [MMWA11]. Drigo [COP16, HS15, dFR15a]. Driven [Coo12, EM16, GB10, KC16, MS12, SPSA11, WR14a, Xu16].
drug [AB16b, BJ17, HM10b, IAK13, KKS+11, MS10, RdPW+12, SD13a, SSTÖ11, SK11, HM10b]. drug-DNA [MS10].
drugs [EAK+10b, GCDNGS12, YINM13]. Ds [OM13b]. DSD [YFY17].
DSD-PBEP86-NL [YFY17]. dT [XLGA12]. dual [EMSB15, WWHZ13, YK13, JLG+12].
dual-level [WWHZ13]. ductile [KG17]. due [ALA15, ZSZ14]. duplex [PPK+13].
during [HSYM11, MNC12]. Duschinsky [Man13]. dyads [MUNZVR12]. dye [AGJ12, BG17, ÇAS13, FM16, FSBA12, cLqFtW+14, MY17, MFB11, MANP17, PMAP12, QJ13, SSS15, WKE17, WWB+14, Zha17].
dy-aggregates [WKE17]. dye-sensitized [AGJ12, FM16, cLqFtW+14, PMAP12, QJ13, SSS15, WWB+14, Zha17].
dyes [AGJ12, BBM17, FM16, FBU+11, JPPA10, JWG+12, cLqFtW+14, MY17, Mas10, PP10, WWB+14, ZSAP11]. Dynamic [AFV12, DLG12, KWLS15, AM13b, Ang10, BL16, CCEGK12, CEFMK12, FKL+12, KYS13, LKJ13, MNS11, RC11, RVO+14, TSH17, TPCJ+12, YKM+15, ZWLC12, dWL14].
Dynamical [AFM+10, BR10, BR16, GWZ+14a, Sko16, ZZ15, EML+11, Igl11, Igl12, KMF+11, NE11, PETB18].
Dynamics [KKH+13, LLM13, MNE+13, PPK+13, SRPD16, SPPT15, TIN13, TM13, BM16, BBB+12b, BR15, CTVA12, CW13b, CLXD15, CAPL12, Dau16, DGR+16, DLZ11, DP11, EAH13, Fra17, FUE+12, GKS10, GVPCK10, HDÖS12, HXX15, HHL+12b, KTI+12, Kaw15, KCC13, KSC15, Kit14, Kit15, Kit17, KF17, KUY16, LW2W13, LPM+11, LKLW11, MADI12, MMG15, Mak15, MSH13, MDC15, MP12, MCARL11, MOE+11, MMBK12, MMT+13, MRS15, MSK+12, MPL+11, MLB+10, MMP11, Nym14, OHDA13, PD11, PP10, PMH+16, PI16, RMS12, RP16, R11t, SMK+12, SIT+12, SPSA11, SMEH15, SIB+13, SHKS15, SLS+10, SKV12, SZ15, SY17, SBL11, TK16a, TpDB12, UT'T13, Viki11a, VGS10, WWHZ13, XZJ+16, Xu16, Yak10, Yak11, YGL+11, YAF+15, YT14, YINM13, YLC17, Zak16, ZPM10, ZZ11, ZGSM15, ZH15, ZCG+17, ZRL10]. dynamics-friendly [MDC15]. dynamics/quantum [BBB+12b, EAH13]. Dyson [DZO11, SOM10].
[CK13, Lad14, PS14, VV13, XTLA14, COP16, HS15, Lun13a, Man16, MBsAg16b, PS13b, Sha11a, Tou13, VUC13, dSSF16a, dFr15a]. \textbf{Editorial} [Bar16, Brä14, Cav17, For17a, LJ16, LV16, MEF +15, Nag16a, Tch13]. \textbf{Effect} [ALRA10, CdLdSC18, Eil14, KP10, KT12b, MFB11, Mit11b, MTS15, RP11a, Sch10b, SYS14, WLZ +12a, YLW +13, ZCZ +12, dOLdV13, BMTT11, BdTG11, BS14, BGL +16, Bra10, BEPZ10b, CNBPr +11, CYLL11, COP16, DKS11, DK13, GWZ +14b, GZMC11, HV11, HSN +11, IGMK11, JN13, JLG +12, Lad14, LSR10b, LZ12, LPOP12, LWL +12, LWW11, MG12, MS10, MSK +12, MPT11, MW15, ND10, OKK10, OA13, PCMG12, Ry12, RMTG11, RRK16, SD13a, SIM14, SAHAA16, SPL14, SK10, TYN13, TJ17, WWL +11, XTLA13, XTLA14, XWCY11, XZJ +16, YRN +11, YKN13, YD17, ZGSM15, ZKFW17, dSSF16b, dSSF16a, dAVdM17, Jan10, JWG +12, ZAE10]. \textbf{Effective} [CEM14, Liu15b, May14, TSvL +16, Vik11b, YHL +13, BCGC12, CCBR +12, Dw13, GbZA10, KUY16, MPTZ13, MZT16, PGGMR10, TG16, Liu16]. \textbf{Effects} [ABA11, BS16, Bla15, KSAK17, LLZ +12, MSRn +11, PETB18, ACF +11, Ali14, AEM +12, BH10a, BSO16, Chr10, CFGC11, DCD11, DPDR11, DWWZ15, DLLA10, EHKD11, EKD12, EEMSS14, EAV16, Fer11, GR11, GBS17, GWM11, GZF13, GR10, Ire12, IROW10, IK14, JA12, KI15, KRG +13, LDKB15, LGHL11, LDW +11, MZLM17, MURR13, MPE11, NG11, NMHPVG12, Oni10, OGvSG18, PCR +11, PWP13, QHS11, RP11b, RFN +12, RS12a, RSN12, RSM12, RdA11, Ril10, Skt15, TK16a, TV13, TFSRM11, TH12, VFCSC17, VSMK13, WDR +11, WLC +17, XX12, XLGA12, XDM +10, YZW +15a, YMY +13, YT14, YFY17, ZH12, ZYL +13, ZBBB17, ZFC12, dCDC +11, dSNBG08, SMK +12]. \textbf{Efficiency} [Cal10, ATPRV11, BDG17, Mai14, THSR13, VRO +12]. \textbf{Efficient} [BL16, KI15, SHW +13, SCBP17, YM14, ZWSF16, ZRLV10, FZH +18, FM16, IIS +17, LCK +16, SGH10, SAHAA16, WXZ15b, ZCZ +16, ZKW17]. \textbf{EGEE} [LG10]. \textbf{Ehrenfest} [KUY16]. \textbf{eigenfunctions} [PMGMR12]. \textbf{eigenstates} [KB12]. \textbf{eigenvalue} [Mit11e]. \textbf{eigenvalues} [Mit11c]. \textbf{Einstein} [DCD11]. \textbf{elastic} [Per10b, UV18]. \textbf{Electric} [SS12, BL16, DB15, EBR11, GV11, KA11, KT12b, PCD14, SMEH15, SMEH16, VRO +12, YSO12, Zha17]. \textbf{electrical} [GKS10]. \textbf{electrodes} [HWH16]. \textbf{electrocatalysis} [MLW16]. \textbf{electrocatalytic} [FFPD16]. \textbf{electrochemical} [NBZG16]. \textbf{electrochemistry} [FFPD16]. \textbf{electrode} [KJ15, Tug13]. \textbf{electrodes} [Che13]. \textbf{electrodynamics} [FNIT16, IFT14, Lin14, Liu15b, Liu16]. \textbf{electrolyte} [DLO16]. \textbf{electrolytes} [MNE +13]. \textbf{electromagnetic} [Bae14]. \textbf{Electron} [Bas11, DZQ12c, DJ18, DSVP15, LC16, LZ10, MT11, PUH +11, PI16, RVPN12, SLG11, VBC +12a, AA11, Ali14, AEM +12, ALRA11, ARH +13, AST16, BLL +13, Ber13a, BL10, BL11, BKM15, Buc10, Buc11a, CMR13, CW13a, CM15, CG12, CH17, CSMZ10, CSTA16, DLCB15, DAA16, DLJT14, DTEMK11, Dil13, DZO12a, DLLA10, Dum12, FYhC11, Fin15, FA17, FMMD +10, GSA11, GTR11, GS10, JdL08, Jan10, Joh17, KWLS15, Kar12c,
Kha16, KPL+17, Kit15, Kri13, Lar10, LCH14, LZZ+11, LWY13, LYL+12, LG12, Lui10, MGK+11, MR12, MW16, MJ16b, MPD+10, MPZW10, MJ11, MNS11, NA14, NBZG16, NAK+17, Nes11, Ng12, NDM+12, NE11, NRGS11, NMV+14, OAT+13, POLV12, PL11, Pir13, RNV+12, RCM10, RAGM10, RS13, SS10, SBMM11, SBM16, SYK+12, SPD+18, SSAM13, SHS+13, SM12, Sit15, SL13. electron [ScBsR+10, SBKJ18, TC12, VF13a, VBC+12b, WWD+15, WH12, XZYS10, YM14, YRN+11, YHLC15, YD17, ZDZO10, ZFS+11, ZSJ14, ZJS13, dA12, dCDC+11]. electron-group [WH12].
electronic [Kri13, KO12, KUY16, Laii1, LL11, LMZY15, LLZ+14, LbV16, LHL+15, LZ10, Lya14, MSG16, MLC+11, MC11b, May14, MMWA11, MUNZVR12, MBA+13, MPZW10, Mil12, MS17, MA11a, MA11b, MMRA10, MJ11, MB13, MPT11, MPTZ13, MM13, MW15, MSRn+11, MCRS16, MC18, NA12, NIT16, NZAVR10, OGvSG18, PE11, PCR+11, PAKA15, PMAPI2, QJ13, QCb+10, RMLPGGHH16, RS12a, RMJ11, RNC+14, RMTG11, Rus14, RMY+13, SRPD16, SR12, SD13a, SB10a, SLS+14, SXS+12, SLS+12, SLSZ13, SIS+08, SRS+17, STOT11, SR11b, SZZ+12, ScBsR+10, SSW16, SK12b, TYN13, TZ11, TV13, TD11, TFB11, TG13, UTTh13, Var14, VPA11, VLFG12, WWC17, WFS13, WJL+10, YZL+10, YZL+11, YZW15b, YH14b, ZQCJ10, Zha10, ZLZ10, ZZR+12, ZCG+16, ZQXP17, ZCP11, dSSF16b, dSSF16a, Bou12b, Lad14]. electrons [BEM12, BM10, BB10, BMB16, Dw13, Ig11, Ig12, ISRK12, KK13, KK14a, Kry12c, Nes10, QCb+10, RP11a, RVP10, RS13, She12].
[NMHPVG12, TH12, TCS10, CDSK12, DPK12, IG11, KKS+11, KRG+13, PK13a, TYN13, ZC+12]. electrostatics [BWE16]. element [OVT+16, SHS+13]. elementary [EMED+12, EMEPD15, SOF+10, Zil14]. elements [AO12b, CW13a, GI10, LX13, NZ13, RRK16, SW10, TMC+13]. eleven [DCFD10]. ELF [Fin14a]. elimination
elliptical [MFLK11]. Elongation
[\text{KdSM}^{+10}, \text{XLGA12}]. else [Kry10]. Elso [COP16, HS15]. elucidating
[Kaw15]. elucidation [SBKJ18]. elusive [SSP14]. elymoclavine [RGS^{+13}].
eloading [BA13, Lan10, SMV11, JLL11]. Embedding
[ABS11, DB13a, QB15, AB16a, GCK^{+17}, HJK14]. emeraldine [RMTG11].
emergent [SMMT13]. Emerging [GP13a]. emission
[BS11, BSO11, CFP^{+10}, LXW^{+14}, ORJ18, PSK^{+13}, dSdS13a]. emissive
[ZKWZ17]. emitting [MUNZVR12, NZAVR10, SHW^{+13}]. empirical
[Hat13]. enantiomeric [LCZL11, QCW^{+12}, WTZ^{+11}]. enantiomeric [LCM^{+11}].
encapsulated [CWL^{+13}, JLL12a, KG08, TPT^{+13}, WW11, ZLWL16].
Encapsulation [RR11]. endic [ZPW16]. Endo [Jal10]. endohedral
[ACL12, JLL^{+18}, MS17, SCTW10, WLZ^{+12a}, WSL^{+11}, YL11].
endohedrally [NW12]. endohedrals [YK11]. ene [IK14, Sat11b].
Energetic [GB13, GAMM10, HM11, HZZW11, Kar15, LCCH10, LL17,
MTS15, SRA^{+11}, TCSD12]. Energies
[CC11b, FDA16, AG10b, AK17, A0LB12, AEM^{+12}, ART08, AZD^{+11},
AST16, BXR^{+13}, BPVDB11, BP13, BAP12, BSS16, BBL12, Ber13c,
BVA^{+14}, Bout12b, Bud12, CPF^{+11}, CWW12, CNBPR^{+11}, CCL^{+16}, CLH14,
CSG14, COP16, DK13, DB11, DHZS11, EMK14, Fin16a, FMMD^{+10}, GST11,
Gra08, Gra11, HJRO13, HF11, HM10b, HFdGC14, HM10b, HM11,
HBM11, ISN13, IK18, Jeo18, JZP17, KKH18, Ky13a, Kin16, KSN^{+10},
KMM16, KPH^{+12}, Sri13, LFF^{+10}, LSR10b, LV12, LWWZ13, LG16,
LG12, LDLAB^{+15}, LV12a, MZB^{+13}, MGK^{+11}, MDC15, MCP10, MHT^{+08},
MA12, McC13a, MOE^{+11}, MOLF11, MIN13, MGD11, MPRCCEG12,
MLB^{+10}, NAI12, N\text{em}14, Ng12, NDP10, NIT16, PML^{+11}, Per18, PP14,
RPVM10, RTGS11, RCP14, RL10, SAS^{+12}, SIM14, SFC16, SGL^{+16},
SCLCPB12, SA11a, SB16, SLZ^{+11b}, SRS^{+17}, SK11, SGC13]. energy
[SZW16, SZA15, SZY17, SC18, TNN16, TBL11, Tou11b, VPA11, Vik11b,
Vyb08, W\text{ag}14, WKE17, WWL17, XZZ^{+10}, YH14b, YLC17, YLYC18, ZS12,
ZRLV10, dHLs12, dSSF16b, dSSF16a, Yu13]. energy-dependent [SK11].
energy-dependent [FMMD^{+10}]. energy-loss [AEM^{+12}]. energy-relevant
[Wag14]. Energy-surfaces [FDA16]. engineering [WCL^{+17}]. enhance
[ZLWL16]. Enhanced
[BGL^{+16}, LLZ^{+14}, Mas14, MS14c, MPE11, SKV12, TFSRM11, TSBSM12].
enhancement [KKT13, KKT14, SJW13]. enhancements [ATPRV11].

Entanglement


event [GI11a]. events [CSS16]. evidence [HV11, WTV+15]. evidences [CG12]. evolution

[BL11, IFT13, IFT14, JL12b, MLV16, RGR12, YSS+10, YSK+12]. Evolutionary [CGG18]. evolving [LSR+13, VIK11b, YY+13]. Exact [GZSMFN16, HR12, HZF12, Kha16, KUY16, RBD+10, RS13, Zak16, AM13b, Eng16, FA17, Hog13, IHG10, Kry12c, LEU+11, MPB11, PT13, SIF+10, Tou11a, FLCHL10]. exact-exchange [SFL+10]. Exactly
[GMGRMP12, PGRMP10, PMGMGR12]. **EXAFS** [LSR + 13].

**examination** [Kan17]. **examine** [KJ14]. **example** [CP10, DMBL16].

**examples** [DLM12, Hop15, JA12, Mai14, Sic16]. **excellence** [MEF + 15].

**exceptional** [LA11]. **excess** [JdL08, YHLC15].

**exchange** [Dw13, Fin16a, PTH11, ATL + 14, AM13b, AGPDZ13, AK11, BHV + 11, BVRM10, CWW12, Eng16, FB17, IHG10, KMK + 16, Kry12c, LZFZ13, LCT14, Lu15, MMM16, MEEA + 13, Mys12, PDR + 14, RPVM10, RFEPP + 16, RLER10, SPTT15, SFL + 10, SFC16, TA10, XZL + 12, MRS15].

**exchange-correlation** [AGPDZ13, AK11, LCT14, RPVM10, SFC16, TA10].

**exchanged** [PvS10, UMS13].

**excimers** [Cas15].

**Excitation** [KyH13a, BVCAP12, BSS16, FMCA11, dDGNB10, IHG10, LWWZ13, LORR + 12, Mas10, MIN13, SZL + 14, WSL11, YH14b, ZGSM15].

**excitations** [CD15, VAT12, VBC + 12b, ZB18].

**Excited** [Cha11, Glu13, ACF + 11, Cam10, Cao17, CHM + 14, CM16, Cor16, GWHH17, IGMK11, JA12, KT12a, KK14b, KKT13, KKT14, LSL + 08, LV16, LP10b, LGZC15, LZ10, MMWA11, MT11, MNS11, MB12, Nes11, NDP10, Nic11, PRPU + 13, PMAP12, SBM16, SR11b, SK12b, Sza13, TTT13, WKE17, YÇÖ11, ZCG10, MQG13].

**excited-state** [ACF + 11, Cao17, JA12, WKE17].

**excitons** [RP11b].

**exclusion** [CM15].

**exhibiting** [Fin15].

**exist** [BN12].

**exohedral** [GB13, WLZ + 12b].

**ExoMol** [TY17].

**expanded** [RLP + 11, WSV10, YS13, MM10].

**expectation** [MC11b].

**Experimental** [CSSK + 12, DDÇY12, EI11, MLPT10, SC12a, AZD + 11, DSH + 13, FPRGMB12, KAOB11, RGS + 13, SC12b, SRASZ16, SJJL12, SBKJ18, TAY11, VMC11].

**experiments** [LRP + 11, WSV10, YS13, MM10].

**Explicit** [BHIP10a, Koc13a, JCC10, MAD12, MK10a, Pir13].

**explicitly** [GBS17, TH13].

**exploitation** [MP11].

**Exploration** [MOE + 11, MBA + 13, WCS + 13, MDP10, MOLF11, NH11, SSP + 17a, Sic16, TDSD12].

**explorations** [WLL + 13].

**explored** [JMX + 15].

**Exploring** [ACF + 11, DCR10, ESBVY12, HJRO13, KB12, PK13a, ZCG + 17].

**explosive** [DGR + 16, LZZ + 13].

**explosives** [YZ13].

**exponent** [HITU16].

**exponential** [GMGRMP12, GH11, GE12b, Hog13, KH10, LLH15, PGMGRM15, PSG17, Roy13].

**exponential-cosine-screened** [LLH15].

**exponential-screened** [Roy13].

**exponential-type** [GMGRMP12, PGMGRM15].

**expressed** [Glu13].

**Expression** [RA10b, Kuv10].

**expressions** [AEÖ12, GZSMFN16].

**Extended** [Koc13b, CLL + 11, DQZF12, Haj18, HBMM11, Ire12, MPMMC + 11, MSOV13, NZ13, WML11].

**Extension** [Kon11, WB17, BAP12].

**extensive** [IM15].

**extensivity** [RS09, RS11].

**extent** [LDBK15].

**External** [Hor13, Bae14, DB15, Glu13, KSC15, Kit14, RS13, TJS17].

**extractants** [VBJK18].

**extraction** [LCH + 11, LCS + 11b].

**extracule** [MT11].

**extrapolation** [LV12].

**extrema** [SRMB15].

**extreme** [Mit11c].

**Eyring** [BR16, BR10].
Fabricio [COP16], face [DMWY11, DLG12], Factor [Tri14, Kan17], factors [Mam13, MK11, SPO+11, TZ11, VLG12], family [WZX15b]. Fan [Roy14], far [Var14], FARMS [MC17], Fast [GFRdG11, PT13, PSC15, SAS+12]. Fayalite [NDM+12], FCX [SZL+14]. Fe/C/S-doped [OGvSG18], feasibility [JS17], features [CD12, DLG12, Pie12, Sch10b, TC10], FeCp [XCY15]. feed [FCC11], feed-forward [FCC11]. FeFe [BGFD14], female [MEF+15], FemEx [MEF+15], femtosecond [HYH+10, MPC10]. Fenna [BSS16], Fermi [ABLT11, CP13, FA17, IROW10, KCDC15, KK13], fermion [FYhC11, Lun13a, Lun13b, Tou13], Fermions [Kle11], Fernando [COP16], fermimagnet [TD11], ferrocene [DAA16], ferrocenium [DAA16], ferroelectric [DMS+10, DLM+11, OCB+10], ferromagnetic [BXR+13], Feshbach [WB17], Festschrift [KN15], few [Mai14], FF [LGW11], fiber [KFY+12], fidelity [Luz11b], field [Bae14, BBB+12b, Bral0, BS01, BN11, CL11, DCD11, DB15, EBR11, FKL+12, Fri12, FSST16, GZF13, GRD11, HSS+11, ISN13, KKH18, KSC15, Kit14, Lc14, LB14b, Mit11b, MPL+11, PVS12, PL11, PCR+11, Pop15, RP11a, SRPD16, SY10, SMEH16, SAHAA16, SR11b, SV11, SHMR11, TVSvL+16, Vik11a, Vik11b, Vik13, Zha17, dAB17]. field-effect [SAHAA16], field-emission [BS01], field-theoretical [Fri12], fields [Bae14, CSS16, FT15, GV11, KT12b, PM12, SRPD16, SMEH15, Stol8, WYM15], film [RAMB18], Filho [COP16, HS15], film [JK12], films [GDM+10], filter [Man16, MBSAG16a, MBSAG16b], Filtered [MPV+11]. Finding [SRMB15, KB12], fine [SCZG12], fingerprint [vLRRK15], finite [CS17, FKL+12, NS10b, PE11, TLC+17], finite-length [PE11], firefly [CZC11]. Firsov [AOLB12]. First [BXR+13, DWX+16, FTB11, Fra17, Jia15, Kan17, KL13, LLL16, LIK15, Per10b, RZG12, RJLP+13, RRB12, TZ11, Wan13, ZWL12, vL13, AFA13, BZBZ13, Bon17, CEFMK12, CC11a, CWW+16, CJOOW11, FSB16, FT15, GXZ+14, IGMM11, KSS12, Kim13, LLM13, LBdV16, MKM11, RD14, RVO+14, TCCI10, TW15, VQA012, VDG13, XWY11, YHL+13, dWLC14, WZC+12]. first-principle [TCCI10]. First-principles [BXR+13, Fra17, Jia15, Kan17, LIK15, Per10b, RJLP+13, RRB12, Wan13, ZWLC12, Bon17, CC11a, CWW+16, CJOOW11, Kim13, LLM13, YHL+13, WZC+12]. first-row [BZBZ13, MKM11]. Fischer [MJ16a], fisheri [PI13]. Fisher [Nag15], fit [Haj18], five [RVN+12], fixating [WR14a], fixed [IM15], flavonols [FZX18]. flavor [Tch16]. flavors [Mat02, Mat10]. flexibility
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Free [AG10b, LCG12, MLB+10, AK17, BDG17, CFOC+10, ENV15, FM16, Fin17, FA17, Kla11, KDA+11, LSR10b, LSG+14, Luz11a, Luz12, LGS+16, Nag15, Rit12a, Rit12b, SX15, TPT+13]. free-radical [LSG+14].

frequencies [MCE11, Rud12, ŞBAT16, SZL+14, WHY+14, YWH+12c].

frequency [MPC10, TU10, ZPZ15, ZLE17].

friend [Sau11]. friendly [MDC15].

fringes [YS13]. frontier [ABA11, LSR+11, YZZH15, LSR+10a].

Frontiers [HKLW13, ISN13, IKN13, Kut13, MIN13, NS13, OHDA13, SIB+13, SHS+13, SKY+13, TKN13, TH13, UYN+13, UTTn13, YKN13].

frozen [Mas10]. FT [ÇAS13]. FT-Raman [ÇAS13]. FTIR [ÇAS13].

fuel [FFPD16, Sic16]. Fukui [Boc17, MJ11, SKL10]. fulfillment [RLER14].

Full [BEM11, Dau16, SR12, YIY+13, DVDBM11].

Full-configuration-interaction [BEM11, DVDBM11]. Full-dimensional [Dau16]. Fullerene [DJB10, CCEGK12, DI15, DFK16, FBO+11, KP11, KK11b, KK12a, MSS11, MS17, Nik11, PAKA15, RR11, RGPZD13, TSK17, Var11, ZW15].

fullerene-buckycatcher [DI15]. fullerene-derived [PAKA15]. fullerenes [ARH+13, DI11, GZW16, JLL+18, LBW11, MNS11, YLZ+17, ZCG+16].

fulleroid [Iku17]. Fully [RTT10, AC12, RVNP12]. fulvene [Val17].

Function [Kut13, NS13, TKN13, TH13, YKN13, AB16a, AO12b, AROL12, BL10, BL11, Gao11, KL11, Kuy12, Liu15a, MRS15, Ng12, OAT+13, RZ17, SGN10, Sta11, SS12, SD13c, Toul1a, UYN+13, WWL17]. Functional [Auo11349, HKLW13, ISN13, IKN13, MIN13, SKY+13, TK16b, AK17, AM13b, AGPDZ13, BMK+14, BD14, BGC12, BVCAP12, BDF+16, BGBV12, BLKB11, BJDIMAV12, CCL+13, CNEK11, CH17, CM12, CZLD17, CK17, CF14, CTDOA10, CSTA16, CD12, DWJZ11, DCCB11, DKS11, DW12, DZ1a, DGR+16, DQZF12, ED16, FCS13a, FCS13b, FZXY18, FO10, FDN10, Fin17, FA17, FS16, GCK+17, GM11, GGD12, GHCCMCQM17, GD11, GCZ+14, HHC10A, HLT+14, HMH10a, HHH10b, HHK113, HYD11, HZWW11, IN15, JR12, JPP+11, JA12, JS17, JW18, Kar13, KK14b, KKL+16, KSAK17, KSG+12, KJ14, Kri13, Kry12c, KG08, KMU+13, Lat13, LPO+12, LSR10b, LW11, LWL+12, LWX+14, LBY+14, LLW+11, LCK+16, LDZG16, LLZ+12, LNI12, MYZ+10, MLW+14, MJ16a, MLC+11, MFK+12, MA10, MW16, MUNZVR12, MG12, MKSG13, MLK17, MLB+12, MBBT+12, MM13].

functional [MKW11, MCRS16, MOH+12, Nag15, Nag17, NDP10, NTLN10, NL11, NMIP14, NMR14, NMD+12, NZAVR10, OD16, POLV12, PS10b, PS14, PI13, PMH+16, PABSK16, PP16, PTH11, PR10b, Pir13, PU14, PJP10, PMP12, PI16, PC13, QHS11, RGPZD13, RS12b, RPVM10, RAMB18, Rud12, RSCS10, SGL+16, SVRGV12, SN12, SAHG11, SHL+13, SIS+08, SDDM12, SRMB15, SK12b, SS13, TOSN12, Tan12, TIN13, Tan13, TBD17, TFZ+15, TLC+17, UMS13, VPGC12, Ven12, VUC13, Vik13, VBO+15, WKE17, WJL+11, WW11, WJY15, WDJ+17, WTZ+11, WR15, XNL+14, XSLF12, XGH+18,
YWH12a, YWH12b, Yu13, YL11, ZT13, ZKKR11, ZQJC10, ZLWY13, ZCX +16, ZR +11, ZMZ13, ZGC +16, ZSZ14, dCSdoMC13]. functionality [ATS +11]. Functionalization [ZWWY10, JNY17]. functionalized [LRKM10, MOV13, MLW16, OD16, SPPT15, TDOD17, WLZ +12b, ZK12]. functionals [AF16, AK11, DCDD10, DCFD10, Fin16a, HFdGC14, Jan13, Jou13, KDOR17, Lai14, LCT14, LSP +16, LORR +12, Lu15, PSMD16, PRFR17, SFC16, SMOD11, SOF +10, SSP +17b, SGC13, SX15, TA10, TCA10, UV18, VSL +15, YF16, YFY17, dSdS13a].

Functionalization [ZWWY10, JNY17]. functionalized [LRKM10, MOV13, MLW16, OD16, SPPT15, TDOD17, WLZ +12b, ZK12]. functionals [AF16, AK11, DCDD10, DCFD10, Fin16a, HFdGC14, Jan13, Jou13, KDOR17, Lai14, LCT14, LSP +16, LORR +12, Lu15, PSMD16, PRFR17, SFC16, SMOD11, SOF +10, SSP +17b, SGC13, SX15, TA10, TCA10, UV18, VSL +15, YF16, YFY17, dSdS13a].

Function [GLT13, IA13, KBF +13, ONK +13, CSMZ10, CML +16, FRGC10, GBS17, GTR11, GS10, HITU16, HG08, Hog13, Hor13, KH10, Kar13, MPV +11, MSNP18, MJ11, NS13, Oht13, PABSK16, SPO +11, SZS +10, SLZ +11c, SLZ +11a, SKL10, VSL +15, WH12, YMI14, vLRRK15]. Functionalization [ZWWY10, JNY17]. functionalized [LRKM10, MOV13, MLW16, OD16, SPPT15, TDOD17, WLZ +12b, ZK12]. functionals [AF16, AK11, DCDD10, DCFD10, Fin16a, HFdGC14, Jan13, Jou13, KDOR17, Lai14, LCT14, LSP +16, LORR +12, Lu15, PSMD16, PRFR17, SFC16, SMOD11, SOF +10, SSP +17b, SGC13, SX15, TA10, TCA10, UV18, VSL +15, YF16, YFY17, dSdS13a].

Functionality [ATS +11]. Functionalization [ZWWY10, JNY17]. functionalized [LRKM10, MOV13, MLW16, OD16, SPPT15, TDOD17, WLZ +12b, ZK12]. functionals [AF16, AK11, DCDD10, DCFD10, Fin16a, HFdGC14, Jan13, Jou13, KDOR17, Lai14, LCT14, LSP +16, LORR +12, Lu15, PSMD16, PRFR17, SFC16, SMOD11, SOF +10, SSP +17b, SGC13, SX15, TA10, TCA10, UV18, VSL +15, YF16, YFY17, dSdS13a].

Functions [GLT13, IA13, KBF +13, ONK +13, CSMZ10, CML +16, FRGC10, GBS17, GTR11, GS10, HITU16, HG08, Hog13, Hor13, KH10, Kar13, MPV +11, MSNP18, MJ11, NS13, Oht13, PABSK16, SPO +11, SZS +10, SLZ +11c, SLZ +11a, SKL10, VSL +15, WH12, YMI14, vLRRK15]. Functionalization [ZWWY10, JNY17]. functionalized [LRKM10, MOV13, MLW16, OD16, SPPT15, TDOD17, WLZ +12b, ZK12]. functionals [AF16, AK11, DCDD10, DCFD10, Fin16a, HFdGC14, Jan13, Jou13, KDOR17, Lai14, LCT14, LSP +16, LORR +12, Lu15, PSMD16, PRFR17, SFC16, SMOD11, SOF +10, SSP +17b, SGC13, SX15, TA10, TCA10, UV18, VSL +15, YF16, YFY17, dSdS13a].

Functionalities [ATS +11]. Functionalization [ZWWY10, JNY17]. functionalized [LRKM10, MOV13, MLW16, OD16, SPPT15, TDOD17, WLZ +12b, ZK12]. functionals [AF16, AK11, DCDD10, DCFD10, Fin16a, HFdGC14, Jan13, Jou13, KDOR17, Lai14, LCT14, LSP +16, LORR +12, Lu15, PSMD16, PRFR17, SFC16, SMOD11, SOF +10, SSP +17b, SGC13, SX15, TA10, TCA10, UV18, VSL +15, YF16, YFY17, dSdS13a].

ART08, Cin11b, LMZY15, MGK+11, MPTZ13, MZST16, PMGMGR12, PBA15, CM15, CM16, Gra11, GdLT12, GE12b, Mit11c, SS12, ZLJ11 generated [PE11]. Generating [AÖ12b, BW15, Fuk12, LLC+11].

generation [CML+16, GFrG11, MML+16, OD12, ZLR15]. generator [AHT12], genetic [AFM+10, CL08], genome [Kuv10].


Geometrical [CSMZ10, GHCMCMQ17, WJL+10, EKN10, KK12a, LL11, MBBT+12, MM13]. Geometries [CSMZ10, GHCMCMQ17, WJL+10, EKN10, KK12a, LL11, MBBT+12, MM13]. geometrical [CSMZ10, GHCMCMQ17, WJL+10, EKN10, KK12a, LL11, MBBT+12, MM13]. geometric [CSMZ10, GHCMCMQ17, WJL+10, EKN10, KK12a, LL11, MBBT+12, MM13].
EMSB15, JLJ+17, KKC14, LJJ+11, LLG+12, LDZG16, LZD+11, LLZ+12, MS14c, Sch13, SMP10, SPI14, SYY16, SCZH16, TL15, VVJ15, WTW+15, XZYS10, YZZ16, ZZL+11, ZLWZ16, ZYL+14, dOdCMuDaLR11.


[Dun15, Kin13, MPRB+10, ZCG10, Beh15, BHH+13, CRFR11, CLH14, CML+16, DSFT17, Fer11, Jeo18, KG17, KMU+13, LCL+10a, clqFtW+14, Luz08, Mai14, MDC15, MiI12, NKKN15, RGTS11, RNE10, SPP+17b, SZL+14, WCGD12, XZZ+10, YYY+12, YZ13, YM14]. high- [Fer11]. high-dimensional [Beh15]. high-efficiency [Mai14]. high-energy [CLH14, XZZ+10]. high-energy-density [Jeo18]. high-harmonic [CML+16]. high-level [LCL+10a, RNE10, SZL+14]. High-lying [ZCG10].


[KPH+12, WZW17, KRH13, LLZaH14, NDH10, OK16, SMEH16, YAF+15]. hill [SB12a, RA10a]. Hillman [ZQQ+17]. hindered [SBEH11]. Hirschfelder [Haj18]. Hirschfelder-long-range [Haj18]. histidine


hollow-caged [PAKA15]. Holstein [DTFK15]. HOMg [LGP+12]. HOMO [MA12]. Homodimers [ZS12]. homogeneous

[CSTA16, Lak10, MLB+12, MMM+12, Sic16, Yak10]. Homology [PTD+12, SLS+10, CSVCB12]. homolytic [KZA+17, OK16, OKR12]. Homonuclear [EMS16, KBGC12, NZ13, SM14a]. HONPAS [QSM+15].


[MMG15]. horseradish [ZST+10]. host


[KBG17, AAH16, HRT12, HYZS12]. hubbard


[Haj18]. Hulthén [Roy15]. Human [CSVCB12, WTH+11]. humans
hybrid-density [SIS+08].
hybridase-lyase [SC12a].
hydration [Ma14, Pat15, PBM10, RGR12, SL10].
hydration [MLW+14].
hydration-lyase [MLW+14].
hydrate [XXbX+13].
hydratase [MLW+14].
hydratase-lyase [MLW+14].
hydrated [BMF+14, EPS+16, MNC12, SMEH16, SCS15].
Hydration [ABS11].
hydrogen [AO12a, BLR12, BAP13, Cha10, CTDOLA10, GZ14, HS15, JLG+12, KK11a, MSVMCI10, MURR13, ND11, NBL12, OA12, PCMGI2, SGKG12, SKM11, YL10, dFR15a, dLRR11, AKHS13, BCCG12, BNI2, BL11, CdLdSC18, CN5K11, CC11a, Coo12, COP16, DAC11, DAC12, Den13, DLG12, DLM12, DLP17, DB15, EK10, EPS+16, FAFR12, FRNM12, FMCA11, FKCI2, GI14, GIO12, GH11, GZMC11, HNH+12, HNBG15, HYD11, IAA15, IK18, JN13, JCCZ12, JZZH17, Kar12c, KKG12, Kry10, LLF+12, LJW+11, LLG+12, LWX+14, MS14a, MdAdCS12, MK11, MK12, MNV+17, MCAL11, MTL+12, MT10, MFLK11, MMBK12, MS14c, MMM+12, MNS11, NW12, NG11, NMP14, NH11, NHB12, NRGI11, NRP+11, NRHI11, NEEV15, OH12, OH13, OHA13, OA13, PM17, Pup11a, RZ17, RJY+10, RJA+10, RYM12, RII10, Rit11, RNE10, RB11b, SRPD16].
hydrogen [SS10, Sch10b, Sch13, SK17a, SMP10, Sic16, SSP14, SPL14, SYS14, SS12, SW12, SCZ16, SCBP17, TL15, UVD10, Var14, VSMK13, WCCD12, WHZ13, WZHZ17, WWLZ17, WJ11, XDM+10, YW11a, YWH12a, YWH12b, YRN+11, YWH+12a, ZAE10, ZZL+11, ZLZ+14, ZL10, dSSC12, dSSF16b, dSSF16a, dFR15b, dAVdM17, dOR10].
hydrogen-bond [OHDA13].
Hydrogen-bonded [SGKG12, CdLdSC18, LJW+11, MT10, OA13, RNE10, ZLZ+14, dSCC12].
hydrogen-bonding [DB15].
hydrogen-bonded [CC11a].
hydrogenase [BGFD14, MG10, DM10].
hydrogenated [IIW+11].
hydrogenation [TGA+11, VPGC12, XSLF12, ZCC15].
hydrogenic [DLRMFY10].
hydrolysis [CCL+10, KFS13, PRFR17, PMC11, RNdA+10].
hydrophobic [NHG+12, SMK+12].
hydroquinone [NP18].
hydrosulfide [HJJ11].
hydroxamicates [TPdMB12].
hydroxamic [KK11a].
hydroxide [RGR12, WZZL10].
hydrides [DCDD10].
hydroxy [TAY11, YLW+13].
hydroxyacetone [SSdS17].
hydroxyanthraquinone [JB11].
hydroxybenzaldehydes [EKN10].
hydroxybenzenes [ATM17, KM12a].
TFZ+15, WLL+13, BGMD15, DGR+16, EM17, KCDC15, MNV+17, MC17, RNdA+10, SAG13, SC11, VHTEG15, YWJ+11, AF16, Tan13. **Insights** [CP13, MS14a, MC18, SLA12, TFBG14, VBO+15, Bal16, DJB10, LXW+14, LKZ+16, MNE+13, NP18, Pan16, SR11a, XZY10, YHLC15, dARAV12, KMS+11, QTCL10]. **instability** [Pat15]. **instanton** [Buc12a]. **insulator** [BEM11, Lar12, SAHG11]. **insulators** [YZZH15]. **Int** [BR16, COP16, HS15, Man16, dFR15a]. **integral** [KSST12, LWY13, Mak15, RCGLV14, SGC13, YK13, ZLR15]. **integrals** [AE¨O12, AA15, GTR11, GS10, Hog10, YM14, YS¸ ¨O12]. **Integrated** [Cap16]. **integration** [BG11a]. **integrations** [Koc13a]. **intelligence** [Ezz10, SRS17]. **intense** [DLCB15, SRPD16]. **intensities** [VVVB10]. **inter** [Tav11]. **interacting** [Cap16, DM12, Dil13, KWWH18, Nes10, RP11a, RS13, SGL+16]. **Interaction** [ASHF13, DWPK14, EG10, JLS13, MYZ+10, MRT11, RNB+10, SPD+18, SK11, TBRIS10, ZT13, Bae14, BLL+13, Bas11, BEM11, Ber13b, CAZ+11, CCL+13, CGM12, CGG18, CRSB12, Cha10, CC11a, CP16, DC14a, DVDBM11, DTVP+12, DLG12, DWZZ15, ELC08, Eng16, EBH11, EAV16, FZX18, GWZ+14b, GD11, HFD11, HM10b, JFT13, JH15, JLG+12, KPH+12, LG+12, LBdV6, Luz08, MMR+10, Mar12, NL11, NV10, NFQ+11, OA12, PSK+16, RYM12, RFN+12, RS11b, RRCO11, SD13a, SD16b, SKHN13, Sha11b, SLZ+11c, SS11, SM14d, SWS12, SLZ+14, SYY16, SCZH16, TK16b, TG16, VHTSG15, VVVB10, WLL11, WZW17, WWQG17, Win10, XHbX+13, ZST+10, ZCZ+12, ZS12, ZMB+17, TBRIS11, TBRIS12, YL10]. **Interactions** [KMMS17, MFK+12, dCDC+11, AGRI+12, BMR+13, BAP12, BLWJ17, BGD17, BWE16, Buc12b, CNBPR+11, CdLdSC18, CNSK11, CCS13, CKL16, Chu12, CSP+10, Cys11, DJB10, Dob14, DLP17, EAA17, EA12, EMS16, FNBK17, FRGC10, FKC12, HYD11, Jal10, JEA13, JLZ+17, KdpPNS16, KMK+16, KPI2, KKG12, Kry12a, Kuv10, LMZ+11, LC16, LZZ+13, LDZG16, LB18, MZB+13, MS12, MSNP18, MDP+10, MPZWD10, MS10, MSY+12, MZL17, MAW+18, MURR13, Na13, NRI15, OA13, PML+11, PABSK16, PP16, Pie12, PETB18, RKA14, Ril10, Riv11, RGR12, Sch15, SSAM13, SM14b, SM14c, SS13, TH12, TDOD17, TCS10, Var11, VBC+12b, VSMK15, Yak11, YJ17, Yu13, YF16, YFY17, Zak13, ZRY+13, ZFS+11, ZLWZ16, dCSDdMC13, dOdCMUdALR11]. **intercalated** [CWF11]. **intercalation** [KKS+11, MS10]. **intercalators** [Net12]. **interchain** [FNBK17]. **interconversion** [AZD+11, SAS+12, Ssd17]. **interdigitation** [MCKD11]. **interelectronic** [ALRA10, WPW13]. **interest** [Sko16]. **Interesting** [KBGC12]. **interface** [DLZ11, LLM13, SFNC+18, MRS15]. **interfaces** [NBZG16, SFL+10, TTM16, WML11]. **Interfacial** [IMS+13]. **interference** [YS13]. **interleukin** [WLL+13]. **interleukin-2** [WLL+13]. **Intermediate** [RMP+14, JL12b, MPRCEG12, Tal11]. **intermediates** [GGZZ16, KZZ13b]. **intermetallic** [AO12a]. **Intermolecular** [EEA17, LZZ+13, MZB+13, Pie12, Yu13, ZRY+13, BPG+10, Buc12b, EML+11, EA12, KP12, MB15, OA13, OD12, PML+11, SPI14, TNN16, Tav12].


involve [Bud12]. involved [CLXZ12, MM10]. Involvement [LSL+08]. involving [LLLB13, Rii10, TCA10, YHLC15]. iodide [MJ14]. iodides [LV15]. Iodine [MOY13]. iodo [LZD+11]. iodo-perfluorobenzene [LZD+11]. ion [ABS13, AB16a, BS14, COP16, DLO16, DCHC11, EHKD11, EK12, FBRBR12, FDMR11, GB12b, GH11, HMI+15, HILJZ1, HFL+17, IAA15, KMS+11, KLK13, KHH10, MS14a, MPTR12, MNC12, Ng12, Oni10, Oni12, SSP+17a, SIZ+10, SLZ+11a, SLS+11, SLZH12, VIK13, WFS13, XLAG12, YW11a, dSSF16b, dSSF16a, SSP14]. ion-covalent [ABS13, AB16a]. ion-neutral [FBRBR12]. ion-pair [SSP+17a]. Ionic

Issue [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, Ano16-29, Ano16-30, Ano16-31, Ano16-32, Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16-37, Ano16-38, Ano16-40, Ano16-41, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano17a, Ano17b, Ano17m, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17y, Ano17z, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano17-27, Ano17-28, Ano17-29, Ano17-30, Ano17-31, Ano17-32, Ano17-33].

Issue [Ano17-34, Ano17-35, Ano17-36, Ano17-37, Ano17-38, Ano17-39, Ano17-40, Ano17-41, Ano17-42, Ano17-43, Ano17-44, Ano17-45, Ano17-46, Ano17-47, Ano17-48, Ano17-49, Ano17-50, Ano18a, Ano18b, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18o, NYA+13, NT15, OSI12b, For17a, Kon10, LV16, Rei15, Sup45a, ÁLVGZW12, Ano12o].


VVAO12, WCY+10, XWCY11, YZ10, YLC17, ZLWL16, ZCG10, dOR10.

MB12, NZ13, NL11, Ols11a, Pul11, SBMM11, SY10, SA11a, SSB12a, SN15, SGH10, SLZ+11a, SHMR11, TKN13, VAT12, WWL17, XLGA12, Xu16, YK113, YSÖ12, ZCG+17, ZL10. **Methodologies** [RSCS10]. **methodology** [CF11, FCC11].

**Methods** [Brä13, Hor13, IFT13, MSH13, Mar13, YK13, ZJS13, dGR14, BLRdA+10, CP10, DGA+13, DFV+12, Exn11, Gag11, HNH+12, Hat13, HJK14, HJ13, JW18, KKH18, Kon10, LP10b, Lya14, MPM15, MC17, Mar12, MBA+13, Mit11c, MMP11, NC11, NDP10, NMR14, Nym14, PDR+14, PL13, Pie1l, RFEGBP+16, RS11b, RSCS10, SGB11, SOF+10, Sch12a, Sza13, SPM+15, Tok16, TG13, UYN+13, Var1l, WHE17, WH12, WCM14, ZX15b, YZ13, YKN+15, YSÖ+12, ZCG+17, ZL10]. **methoxy** [BLM+12, KAOB11]. **methoxyalkyl** [BLM+12]. **methoxyphenol** [KAOB11]. **methoxyphenyl** [ZSASS13].

**Methyl** [SC12a, SC12b, CMCN11, DDC¸Y12, 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]. **methylacyl** [LZZ12]. **methylallenoate** [LLF17]. **methylamine** [LLZZ10].

**methylation** [BS14, CAAI12, WYWL13, YPDW14]. **methylbenzylidene** [TAY11]. **methylcyclobutyl** [KDC¸12]. **methylcyclohexylidene** [KGVG11].

**methyldiazonium** [BS14]. **methylene** [ES17, MHT+08, Met11, RJY+10, RRVJ10, KAOB11]. **methyloxaziridine** [CPL15]. **methyloxirane** [CPL15]. **methylphosphonate** [HYZ13]. **methylsulfonyl** [SK14].

**Mexican** [ÁIGVZW12]. **Meyer** [WCGD12]. **Mg** [BLL+13, PAKA15, TW10, WCY+10, XZZ+10, YLW+13, BJ17, CRB+12, DTEMK11, SC11, dOR10]. **MgB** [PK13b]. **MgC** [LSZ12]. **MgH** [HSYM11]. **MgO** [SAHG11, SAHA12]. **MH** [BLL+13]. **Micelle** [KMT+12]. **Michael** [DP12, PDNC14, SHL+13, WZZL10]. **micro** [RAK10]. **micro-** [RAK10]. **microequilibrium** [SGB11]. **microhydration** [MTS15]. **microiterations** [MOLF11]. **microkinetic** [Tan13]. **mixed** [MCP10, PBM10, SRS+17]. **minimal** [Lai11]. **mise** [Kry10]. **mise-en-scènes** [Kry10].

**mixed** [CP11, DK11, FFDR10, KL11, KSY+11, Lai14, LJW+11, ST15, SN12, TPCJ+12, XTLA13, XTLA14, YY+13, YSK+12]. **mixed-quantum** [CP11]. **mixed-quantum/classical** [CP11].
mixed-valence [FDNR10, KSY+11, TPCJ+12, YYY+13, YSK+12].
mixtures [HFL+17]. Mk [NYS+10, SKHN13]. MK-4965 [SKHN13]. MLi
[SM17]. M’M [MLY+16, AMMK11, Cap16, DGM10, Exn11, GFRdG11,
MOLF11, MG10, RNC+14, SDP+16, SD16a, SD16b, ST15, SLA12, UYN+13,
VATEG15, ZKW17, dAGNJ12]. MM-ER [TIKN11]. MM/continuum
[Cap16]. MMPs [TPdMB12]. MN [PAKA15, BXR+13, BDR12, YL11,
KLK13, MRT11, PM17, SAHA12, TMM+14, YYI+12]. Mn-superoxide
[PM17]. MnX Mn [YIY+13]. MO
[ZLY+14, MLY+16, MGP16, BB10, Bou12b, Na13, DWPK14, GD11]. MoB
[DJ95, DJ12, LYD+18, PVS12, SSt10, ST15, SD12]. Model
[LEU+11, AMAM18, BPL13, BMG14, BKM15, BH10a, Buc11a,
Buc11b, CPF+11, Cam10, Cam12, Cap16, COFC+14, CNSK11, CSVCB12,
Cys11, DZO12c, DQZF12, FMP+17, FB17, FS11, GLOGM+11]. modeled
[MMBK12]. Modeling
[BRS10, IBA+11, Kry12a, LBM11, Men15, MRÅ11, NBZG16, Pog12,
TCM+12, ZPZ15, BGFD14, Buc10, CRSB12, CSSK+12, DFK16, DLM+11,
DFF+12, FBO+11, KMS+12, LZZ12, Mai14, MPJ12, MCV11, OTV+16, PTD+12,
SJZL12, SLS+10, SBKJ18, SM14a, SSb+12b, TAY11, YBMK12, YJ17,
ZP16, ZK12, dAGNJ12]. Models
[FFF10, AM13a, BMR+13, BM16, Buc12b, CWW12, CPAT11, CSTA16,
EPS+16, FvLA15, GMT16, JCC10, KO10, LvdSm14, Li15, LORR+12,
LWH+12, LZ10, Luz13, MPV+11, NS10b, PI13, PL11, RFEGPP+16, SKT15,
SJV13, TD11, VLG12, WYM15, YYI+12, vLRRK15]. modern [Hat13].
modes [CLXZ12, FKC12, PM12, RPBB11, RA10a, TUI10]. modification
[Wan11]. modified [DJ18, HFF12, LZW+15, PSK17]. modulated
[HGB08]. Modulation [MS14a]. MODYLAS [YAF+15]. Moeller [EG10].
MOFs [PK16]. moieties [Cha11]. moiety [BS14, ELCO8, SKM11].
Moiseyev [Brä12]. Molecular
[Buc11b, CSS16, CSSK+12, CHV14, DGR+16, DLZ11, FU+12, Hor13,
IHG10, KTT+12, KM12c, KKT13, MY17, MAD12, MSH13, Mar13, MP12,
MOY13, McC13a, MMT+13, NV10, OHDA13, OA13, Psv10, PWH+12,
PPK+13, RAK10, SMK+12, STT+12, SVPTM+10, SIB+13, SHS+13, SSS15,
TPdMB12, UYN+13, UTn13, VATEG15, WML11, WBP+14, YK13,
YINM13, dSSdG12, ABA11, AA15, Bae14, BL16, BBB+12a, BPT12,
BDF+16, BMF+14, BMB10, BBB+12b, BR15, BWE16, CRA+11, CDSK12,
Cam10, CZ12, CTV12, CCL+16, CD15, CNSK11, CAPL12, COP16,
Dau16, DDCY12, DMWY11, DLY12, DDF+12, DdG+11, DWG12, E14,
FZH+18, FRRB12, FMP+14, For12, Fra17, FUB+11, FSST16, Fuk12,
molecular [JdL08, Jan10, KLK13, KCK14, KHH10, KKH+13, KKT14, Kry12a, KRG+13, KUY16, LB14a, LG10, Lai11, Laz14, LLM13, LA11, LItdSJ+10, LFS+11, LJSS12, LKW11, LNI12, LB18, Ma14, Mam14, MC11b, MHT+08, Mas14, MOE+11, MMBK12, MKSG13, Mit11a, MSY+12, MSK+12, MPL+11, MBTVR12, MBBT+12, MMP11, Mur12, NKKN15, NDH10, NAK+17, Nic11, Nik11, OT14, OWD18, PP10, PMH+16, PBI12, PBB15, Pog12, PETB18, PRG+10, Puz16, RS12b, RSM12, RP16, RLER14, Rit11, RC11, RAMP18, RdPW+12, RA10a, SC12b, SLZ+11b, SXS+12, SLS+12, SLSZ13, Shi13, SRS+17, SLS+10, SKY+13, SWS12, TK16a, TY17, TFA10, Tok16, TSH17, TIKL13, TC12, Vik13, WZ10a, WFS13, WC14, XFW+14, XXJ+16, Xu16, YZZH15, YAF+15, YT14, ZSASS13, ZFW+13, ZPR10, ZLE17, ZLW16, ZRV10, ZB18, dSSF16b]. molecular [dSSF16a, dOdCMUdALR11, dWLC14, dOLdlV13, vL13, vLRRK15, Puz10, RdA11]. molecular-dynamics [PP10]. molecular-level [Shi13]. Molecule [ANC+15, AM12, ASK15, Ber13c, CAZ+11, CL11, CHM+14, CHM+17, CC11b, Cor16, DAC11, DAC12, DAR+11, DPRK12, DLG12, DCZ17, ES17, Fra17, GWHH17, GI11a, GT13, HK11, IIS+17, KKH18, KSC15, KP12, KN15, Lan10, LJSS12, LEU+11, Luz11b, MGG11, MHT+08, MSS11, MZLM17, MPTZ13, MC18, OT14, PK13a, RPBB11, SXS+12, SLSZ13, SLZH12, SRA+11, TFBG14, TH12, Vik11a, Vik11b, WR14a, YW11a, KRC+16, TFSRM11]. Molecule-adapted [ANC+15]. molecule-TiO [TFSRM11]. molecule-to-material [TFBG14]. molecules [Agb12, Ale13, ACL12, BMK+14, BdTG11, BCHN16, BRS10, BDG17, BBB16, BB10, Can12, CM17, CPL15, CRSB12, CK17, CF17, DIOG12, DK13, DSRGD12, Di13, DCR10, EML+11, EMS16, GFB12a, Gin10, GS11, GHP11, HRT12, HMH+13, HST13, HNBG15, HYH+10, Jen13, JMY+15, Jeo18, JZP17, JCCZ12, KBGC12, KBG17, KKL+16, Kim16, KKH+13, KKS+11, KKT14, LKDC11, LPM+11, LLP17, Luz12, MSG16, MCE11, MK10a, Mar12, May14, MFLK10, MCL11, MSM16, Mit11a, MB15, MJ11, MCK17, MPE11, Na15, NS10b, OKK10, OA13, OD16, PL11, PKK14, PWP13, PB10, Puz16, Puz17, RGTS11, RC11, Roy14, RAK10, SGB11, SD16b, SSS12, SA11a, SKG11, SMEH15, SB16, SMR14, Sto18, SY16, Sut12, SCZH16, SV11, THL+15, TK16b, TH12, Tou11a, VO11, XHZXXZ10]. molecules [YZZ16, YD17, ZS11, ZDF13, ZP16, ZCC11, ZSL2, dSCC12, dSTH17]. Møller [RS11a, BVA+14, NMP14, RS09, TH13]. molten [BM10, DLZ11]. moment [AM12, Ber13c, BVP14, HK11, KSG+12, Kri13, MdAdCS12, YSØ12]. moments [AM10, Ber13a, DPRK12, GFB12b, GI11a, GI11c, MD11, TW10]. momentum [ALRA10, AKR12, MOY13, TCG17, TÀ10, YOS15]. Moniliophthora [PTD+12]. mono [Buc12b, Jac12, MMR+10, PS13a, ZQXP17, BL10]. mono- [Buc12b, Jac12, MMR+10, PS13a]. monoacetylides [DD17]. monoamines
66

[MBTVR12]. monoatomic [Bar11]. monoboronyl [MLK17].
monobromide [HTM10]. Monochloride [MOY13]. monoclinic [DWX+16].
Monofunctional [XZ11]. monofurazan [ZZX10]. monohalogenated
[MMV+17]. monoiodide [HTM10]. monolayers [MDP12, RZC13, TTM16].
monolithiated [WWL+11]. Monomer [Cas15, JWJ+12, MM13, BMR+13].
monomeric [Rua10]. monomers [MBA+13, UJSJ13]. Monometallic
[ZW15, GZW16]. monomolecular [MOSK10]. mononitride
[DSH+13, HFD11]. monooxygenase [SSI+10]. monophosphates
[FAK+10]. monosulfur [WJ11]. monovinyl [dlLIA+12]. monoxide
[AKC10, Hog13]. monoxides [TG13]. Monte [AVF12, ABG12, ANC+15,
ASK15, Cal10, CP16, Hog13, HMI12, JCCZ12, PDR+14, RCGVL+14,
SCG13, SCBP17, Wag14, WCM14, ZLR15, ZCC11]. montmorillonite
morphine [RCM10]. Morse [Agb12, PSGK17, Sta10, Tou11a, ZLJ11]. most
[GI10]. motif [SLZ+12, YD17]. motifs [Kry10]. motion
[Cam10, DKR10, KDC15, MMCN+11, SRPD16, Sut12]. motions
[XXJ+16, YW11a]. motors [OWD18]. moving [FAFR12]. MP2
[KBMM10, LKLW11, NMP14, yOITn15, RSM12, SZ11, Tav12, Yu13].
MRCC [NYS+10]. MRCI
[DAR+11, LJSS12, Mit11a, ONBP11, SLZ+11b, SLZ+11a]. MRPT2
[KKT13, KKT14, Koc13a]. multi-center [Koc13a]. Multi-component
[KKT13, KKT14]. multiband [PK13b]. multicenter [CwCW+11].
Multichannel [DS12, SD12]. multicharged [MGK+11]. multicolor
[CYLL11]. multicomponent [Kar13, OT14]. multiconfiguration
[DCHC11, LCL+10b, LPG+12, SL13]. multiconfigurational
[Gag11, HJK14, KK14b, Luz13, NS13, PP16, Pie11, SY10, VRM11].
multidimensional [Kha16, SIB+13]. multielectron [Kry11b, Kry12b].
multieexcited [SCZG12]. multimode [RGPZD13]. multiobjective
[SSB12a]. multiparameter [GGRMP12, IIH16]. Multipartitioning
[RS09, RS11a]. Multiphoton [NWQX11]. Multiple
[HHGqZZ17, PBM10, PP14, DB12, GFRdG11, Ish14, MNV+14, YGLL10].
Multiple-pathways [PP14]. Multiplets [BMB16]. multiplicities [Nal12].
multiply [HDOS12]. multiply-valued [HDOS12]. Multipole
[Tal11, LBW11, YS012]. multipoles [TH12]. Multireference
[CYLL11, LP10b, SWS12, BVP13, GSAY11, HFD11, JNZ+14, Kon10,
MdAdCS12, SLZ+11c, SZL+14]. Multiscale
[Mas14, ZP16, CLKD15, CwCW+11, MGN14, TTM16]. Multistep
[SAS+12, Sic16]. multitopic [SSP+17a]. multivacancy [MF18].
multiwalled [MNS11]. multiwavelet [HS11a]. munnochrome
[GHCMMQ17]. muon [RAGM10]. muscimol [Ser11a]. mustard
[VSMK15]. mutagenesis [CSVCB12]. mutagens [MLPT10]. mutant

[HLMO11]. NBO [DP16, GWZ\textsuperscript{+}14b, NRHJ11, RJY\textsuperscript{+}10, RJA\textsuperscript{+}10, UDVD10]. NC [EMSB15, EMS16, LZZ\textsuperscript{+}11]. NCO [PTS\textsuperscript{+}11, DDF\textsuperscript{+}12]. NCS [Qu13]. ND [ZHI12, BB10]. NdF [SSW16]. Near [MPB11, IAA15, KYS13, ZQCJ10, dARAV12]. Near-exact [MPB11]. near-infrared [dARAV12]. near-IR [ZQCJ10]. near-resonance [KYS13]. neat [AMMK11]. need [MR11]. Negative [DSC\textsuperscript{+}11, IAA15, Kry10, MMRRA10]. negatively [DCBB11, KWWH18]. Neopentyl [MML\textsuperscript{+}11a]. nested [Cal10]. Net [RLZ12]. netted [DW12]. network [Beh15, BGKK16, FCC11, MDC15, WZX15b, dAVdM17]. network-based [MDC15]. networks [CRA\textsuperscript{+}11, CL08, LFF\textsuperscript{+}10, MPD\textsuperscript{+}15]. Neural [BGKK16, MDC15, Beh15, CRA\textsuperscript{+}11, CL08, LFF\textsuperscript{+}10, WZX15b]. neuraminidases [YWY\textsuperscript{+}12]. neuropeptides [dSSdSGJ12]. neurotransmitters [RZG12]. neutral [BCGC12, BGMD15, CAZ\textsuperscript{+}11, EPS\textsuperscript{+}16, FBRBR12, Gra11, MMRRA10, ONBP11, PSSP11, TCN\textsuperscript{+}12, Val17, ZQCJ10]. neuron [CD15, Kar12c, Zag11]. neutrons [Kar15]. News [BDF\textsuperscript{+}16, BHH\textsuperscript{+}13, CYC\textsuperscript{+}15, DOE\textsuperscript{+}14, FMPM\textsuperscript{+}14, KRC\textsuperscript{+}16, LCZL15, MRL\textsuperscript{+}16, MRS15, RRRVJ10, RB11b]. NH [SMC18]. NH-tautomeric [CCL\textsuperscript{+}10]. NHC [Pan16]. NHS [NRP\textsuperscript{+}11]. Ni [AO12a, YL11, AAA12, BXR\textsuperscript{+}13, FBD\textsuperscript{+}13, GP13b, GZMC11, LWX\textsuperscript{+}14, MRT11, SLZ\textsuperscript{+}12, WJL\textsuperscript{+}10]. Ni-based [GZMC11]. Ni-loaded [LWX\textsuperscript{+}14]. nickel [DZO12a, SDR\textsuperscript{+}13, VSMK13, TFA10, dCSDdMC13]. Nicolaides [Ban12]. Nicotinamide [MDP12]. nicotine [SGKG12]. NICS [XWC10]. Nikolai [Pup11b]. Nile [FBBA12, MRA11]. Nimrod [Brä12]. nitramines [MOSK10]. nitrate [HM11, ZL10]. nitrates [HZZ15]. nitration [LLW\textsuperscript{+}11]. nitric [BGMD15, MNE\textsuperscript{+}13, ONBP11]. nitride [Che13, DHZS11, ES17, FZX18, GWZ\textsuperscript{+}14b, Gammad10, Ish14]. nitrile [CMCN11, NAK\textsuperscript{+}17]. nitriles [RFN\textsuperscript{+}12]. nitrites [BL10]. nitro [CL12, GBL10, ZCC11]. nitroaniline [KC11]. nitrobenzene [SS18]. nitroethylene [BBAL12]. nitrogen [BSO11, EAV16, GZ14, HZG12, HNBG15, LZW\textsuperscript{+}15, MS14b, PPdF11, RD14, YZZ16, ZKKR11]. nitrogen-containing [HZZ15]. nitrogen-doped [HNBG15]. nitrogen-heterocyclic [GZ14]. nitroguanidine [DGR\textsuperscript{+}16]. nitropyridine [KC11]. nitroso [YRN\textsuperscript{+}11]. nitroso-oxime [YRN\textsuperscript{+}11]. nitrosodiols [XHZXXZ10]. nitrosoureas [CZJ12]. nitrosothiols [XHZXXZ10]. nitrous [HZG12]. nitrous [BL11]. NMR [AM13a, BMF\textsuperscript{+}14, CAS13, CSP\textsuperscript{+}10, CDT12, EKN10, FBD\textsuperscript{+}13,
OPP°+14, ÖEDB11, Ped16, RRK16, SK10, TTM16, TSK17. NO
[ESS13, LLC°+11, SSAM13, ÁFV12, BAMA12, Les12, MCV11, RNB°+10,
SK14, SSAM13, VLM°+10]. noble
[GI14, JEA13, KDO17, MB15, PSK°+16, SMCh18]. nodal [CSMZ10]. NOF
[PM16]. nomenclature [Tch16]. Non
[BPL13, Cor16, DKS11, SGL°+16, Bra°12]. non- [DKS11]. non-autoionizing
[Cor16]. Non-Born [BPL13]. Non-Hermitean [Bra°12]. non-interacting
[SGL°+16]. Nonadditive [BW18, Cys11, RSN12]. Nonadiabatic
[LKd°+16, WDR°+11, YT14, AC12, HKLW13, IHG10, PM12, SBL11, ZH12]. nonadiabatically [Kit14]. nonbond [BLWJ17]. nonbonded
[ZFS°+11]. noncollinear [GEL18]. Noncovalent
[GR10, MJ11, RLER14, BPL13, BJ12, CG12, Cyb11, DVDBM11, FKL°+12,
MZB°+13, Mam14, MVC13, NS10b, NB17, SPSA11, ZPM10, ZP16]. nucleic
[Kuv10, TBST10, YDW13, ZDZO10]. nucleobase [ZKWZ17]. nucleobases
[Bib13, GGJD13, Kon11, MK10a]. numbers [MHHPR°+17, MKM11]. Numerical
[HV11, JW18, AEÖ12, BKM15, CLC10, HYZS12, MM10, Sit15, TD11, Zak13, RW11]. numerically [GFW11]. nutshell
[BW13a, BW13b, Rup15b]. nystatin [VGS10].
parametrized [Oht13]. parent [MR11, PGG12]. Part
[Bau12, GI11b, Mor13, BR08, BR12a, For12, GI11c, RB08, RB11a]. Partial
[MCKD11]. partially [AA11]. Participants
[Ano12r, Ano10a, Ano10b, Ano10c, Ano10d, Ano11d, Ano11c]. particle
[ATPRV11, BPL13, DTF+11, FMPM+14, Kon11, MGM11, SK17b, VATPR11, VAT12]. particles [ZJS13]. particular [MT10]. partition
[Tou11a]. Partitioning [Vyb08, Ols11b]. partner [MPB11]. partners
[KB12]. Passage [Zak16, Sat11a]. passion [Pup11b]. passivated
[GMT16, SS18]. passivation [MSVMCI10, TCCI10]. Path
[RCGLV+14, YK13, KSST12, Mak15, SGC13, WB17, ZLR15]. path-integral
[ZLR15]. pathogenic [KRH13]. pathway [KRG+13, ZJC+13]. pathways
[ASD14, JL12b, MJ16a, PP14, RBZ15, SYK+12, TKS11, VC13]. pattern
[BS14, CD12, GPM+15]. patterns
[BS14, CD12, GPM+15]. Pauli
[CM15, CM16, Fin15, Fin16b, FDA16, Nag10, PM16]. Pb [NFQ+11, Per10b].
PBEint [FCS13a, FCS13b]. PBEP86 [FY17]. PCM
[AMMK11, PS10a, VSN+11, XX12]. Pd [Bal16, BDFM10, BGMD15, DZ11a,
penetrating [KMT+12]. penicillamine [MVG18]. pentaaqua
[dCSDdMC13]. pentacene [MIN13, IMS+13]. pentacene/C
[MIN13, IMS+13]. pentacoordinate [Yam10]. Pentagon
[KK11b]. pentagonal [WZ10b, Yam10]. pentahalogeno [ZFC12]. pentapeptide
[MRT11]. pentazolides [XZZ+10]. pentoxide [Den13]. peptide
[CF17, FMKJ14, KMT+12, MAW+18, QZH13, QTCL10, SSK11, Sch10b]. peptides
[KyH13a, MAD12, MLB+10, SW12]. perfluorobenzene
[LZD+11]. Performance
[DCDD10, LORR+12, LD2G16, RAMB18, Zak13, AM13b, BHH+13, DCFD10,
DGA+13, FV11, FB17, eLqFtW+14, LZZ+13, Mar12, NKKN15, dSdS13a].
performances [TCA10]. perhalogenated [YZZ16]. perhydroxyl [YM13].
Pericondensed
[BR08, BR12a]. Periodic
[BCHN16, DMBJ15, Fuk12, Gar08, GMT16, GI10, KBGC12, Kut10, LPO+12,
MMA10, NL11, SW10, Tan13]. periodically [Xu16]. Periodicity
[IKS08, HST13, KSI10]. permeability [Pit12]. perynniosa [PTD+12].
perovskite [Oni10, Oni12, OH12, OH13]. perovskites [Kan17]. peroxidase
[ZST+10]. peroxides [FMC11, NEEV15, SSP14]. peroxides [LdMCdA+12].
peroxotungstates [ZLY+14]. peroxo [BCS+12]. peroxycetyl [ZL10].
peroxynitrite [ASD14]. Persilacyclacenes [KAG08]. persistent [SMR14].
Perspective [Ale13, AST16, CM17, GEL18, GRD11, Jen13, KJ15, Lev16,
Mag14, Mas14, MGP16, PU14, Pop15, Puz16, Puz17, Sha11b, Sic16, Sko16,
Sto18, GE12a, JNY17, JMX+15, Jia15, KJ16a, KJ16b, Ols11a, Per18, PP14,
Pull1, Tap15, XXJ+16, ZSZ14]. Perspectives
[Blo15, BT15, Dob14, HJK14, IAK13, Jan13, JNZ+14, KO14, Kaw15, KJ16b,
KJ14, Lin14, LG15, Mak15, MGN14, May14, Men15, MSM16, Nal15, Ném14,
NTCK13, Nic14, PK16, RP16, RNC\(^{+14}\), Rus14, SN15, SX15, Sza13, TFBG14, Tok16, Wag14, WYM15, ZLR15, ZLWY13, Zil14. **perturbation**
[BDPT12, CEFMK12, DK13, DB11, DB13a, DCHC11, JNZ\(^{+14}\), Kry12a, LCL\(^{+10b}\), LPG\(^{+12}\), Lin14, MS13, PBB15, RS09, RS11a, Vai11]. **perturbations**
[BD12]. **perturbed**
[Cal10, PVS12].

**perturbations**
[DB12].

**perturbation**
[BDPT12, CEFMK12, DK13, DB11, DB13a, DCHC11, JNZ\(^{+14}\), Kry12a, LCL\(^{+10b}\), LPG\(^{+12}\), Lin14, MS13, PBB15, RS09, RS11a, Vai11]. **perturbations**
[BD12]. **perturbed**
[Cal10, PVS12].

**perturbations**
[DB12].

**perturbation**
[BDPT12, CEFMK12, DK13, DB11, DB13a, DCHC11, JNZ\(^{+14}\), Kry12a, LCL\(^{+10b}\), LPG\(^{+12}\), Lin14, MS13, PBB15, RS09, RS11a, Vai11]. **perturbations**
[BD12]. **perturbed**
[Cal10, PVS12].

**perturbations**
[BD12].

**perturbation**
[BDPT12, CEFMK12, DK13, DB11, DB13a, DCHC11, JNZ\(^{+14}\), Kry12a, LCL\(^{+10b}\), LPG\(^{+12}\), Lin14, MS13, PBB15, RS09, RS11a, Vai11]. **perturbations**
[BD12]. **perturbed**
[Cal10, PVS12].

**perturbations**
[BD12].
polymer [DI15, FZH$^+$18, MM13, PETB18, SPPT15, Wan11, YT14].
polymerization [AMAC12, CL08, LSG$^+$14, LKZ$^+$16]. polymorphism
[GP13a, PAD$^+$10]. polymorphs [Gao12, VVS$^+$18]. polynitrodiazoles
[RGT12]. polynitrogen [THL$^+$15].
polynitrotetraazaoctahydroanthracenes [ZL12]. polynomials
[Rom10, RA10a, SMOD11]. polynuclear [OPF11]. polynucleotide
[Yak10]. polypeptide [MCE11, NRI15, PCML08]. polypeptides
[YSG10]. polypropylene [Ire12, MLB$^+$10]. polyprotic
[BMK$^+$14]. polypyrrolic [ZQXP17]. polysulfides [YSA$^+$11]. polyyne
[Li15, LORR$^+$12]. population [DFV$^+$12, PM12, VGS10, da12]. populations
[GFRdG11]. porous [GZ14]. porphine [Joh17]. porphyrazine
[HM10a]. porphyrazines [ZAP11]. porphyrin
[MY17, VSN$^+$11, ZSASS13]. porphyrins
[CMR13, CJSNL11, GLPA10, MSOV13, QJ13, TTD13, VC13, Yam11].
portis [CodF$^+$11]. Pöschl [HR12, HFZ12, JZP17]. posed [BMB12].
Post [YOS15, ALRA10, KPL$^+$17]. positions [SY10]. Positive
[FRBR12, MMRA10]. positron [KKT13, KKT14, OT14]. positronic
[GS11, NGS11, ZS11]. Possibility [Sat11a, DMBL16, ZCX$^+$16]. Possible
[MFM18, POLV12, SYK$^+$12, BMF13, KKC14, Kar15, LDZG16]. Post
post-second-order [MSNP18]. pot [LW15]. potassium [Ish14].
potency [DKZ$^+$10]. Potential [BAP12, Ber13c, DHZS11, LDADB$^+$15, McCI3a, SB16,
XZ$^+$10, ZLR15, AB16a, AAHN16, Agb12, AOLB12, ART08, ATY15,
BPVB11, BP13, CDSK12, CNBPR$^+$11, CSS16, DTVP$^+$12, DB12, EMK14,
Fin15, Fin16b, FA17, FB17, FMMD$^+$10, FBU$^+$11, FNI16, Fuk12, GSZ10,
Glu13, Haj18, HDOS12, HR12, HYZS12, HJRO13, HNBG15, HFZ12, IIH16,
JZP17, KMRG13, KMM16, KRG$^+$13, LFF$^+$10, LV12, LKJ13, LDZG16,
MPD$^+$15, MDC15, MCP10, MOE$^+$11, MOLF11, MGD11, MPRCEG12,
MPT11, MPTZ13, Nag10, NMI14, NMHPVG12, PGGRRM10, PML$^+$11,
PVS11, PM16, PKK$^+$16, PSGK17, QD10, RSL10, RCP14, RDM$^+$11, Roy14,
Roy15, Roy16, RS13, SAS$^+$12, SCLCPB12, SMOD11, SMV11, ST15, SRS$^+$17,
SII4, SQ15, SDL$^+$15, SZY17, TNN16, TG16, TSL11, TPDMB12, VPA11,
Vik11b, WKE17, WZX$^+$15a, WC14, YOS15, YYW11b, YLC17]. potential
[YLYC18, ZSAP11, ZLJ11, ZHF12, ZRLV10, Bud12, Yak11]. potentially
[CWL$^+$13]. potentials [AGJ12, BW18, BC15, BC16, Beh15, BBA$^+$16, Cal10,
EI11, ESS13, GMGRMP12, GH11, HI13, KH12, KWW18, Kry12a, KGK13,
LP10b, LLH15, MMM16, MZT16, MB11, PDR$^+$14, PMGMGR12,
PGMGRM15, PM16, Roy13, TH12, Tug13, VLG12]. ppy [ZQJW13]. PR
[DPDR11, GWM11, OPP$^+$14, WLG$^+$11]. practical [RAMB18, SIM14].
prebiotic [VFCS17]. precision [Kin13]. precursor [SSTO11]. predict
[TFA10]. predicted [Jeo18]. Predicting
[DWX$^+$16, KRK$^+$17, PO15, CFOC$^+$10, TWR15]. Prediction
predictions [Bou11, Bou12a, KKH18, TKSK17].

Preface [ACL10, ABC12, Ano13-49, BSS14, DC10, DBMPB11, HLSD14, HB18, NYA+13, NT15, Rei15, Rsv10, Rup15a, RA10b]. preference [EAH13, JN13]. preferences [KM12b, LB18, MAW+13, NRS+11, NJA].

properties/activities

properties

property

property-specific

proportions

proposed

propyl

protection

protein-coupled

protein

protic

protochlorophylide

protocol

proximate

PS

Pseudo
[GFB12a, QZH13, Mit11a, VDG13, ZZL+11, ZFC12]. pseudo- [ZZL+11],
pseudo-10-fold [VDG13], pseudo-Jahn [ZFC12]. pseudo-natural
pseudoharmonic [YOS15]. pseudopotential [Ber13a]. pseudorotation
[ZFC12]. PSII [SYK+12]. Pt [Bou12b, AFV12, KF17, LLL16, MMBK12,
PP10, PRPU+13, YZL+10, ZLLS10, ZCW16]. PtAu [CTW12]. pterin
[JCC10]. PtPd [XGH+18]. Pu [PKK10, PRPU+13, YZL+10, ZLLS10, ZCW16].
puckering [WDSL14]. pull [DSRGD12]. pulses [DLCB15, HYH+10, SVPTM+10].
pure [HDQ+13, SHMR11, TÁ10]. purely [FT15]. purification [KJ16a, KJ16b].
pyrazinamide [SD13a]. pyrazine [NBL12]. pyrazol [TAY11]. pyrazole
pyrrol-2-ylmethyleneamine [LYW11]. pyrrole [BS16, CCS13, CZLD17, PPK+13].
pyrroles [IUMVB10]. Pyrrolidine [PMAP12, KDC¸12]. Pyrrolidine-based
[PMAP12]. pyrrolopyrimidines [dOdONM12]. pyruvic [VF13b]. pz [HHL12a, HHL14].

Q [VF13a, WB17]. QB3 [CFOC+10]. QC [MFLP12]. QC-DMRG
[MFLP12]. QC-simulated [Eil14]. QCTFF [Pop15]. QED [IFT13]. QM
[RNC+14, AMMK11, Cap16, DMG10, Exn11, GFRdG11, KI15, MFF11,
MOLF11, Men15, MG10, SDF+16, SD16a, SD16b, ST15, SLA12, TIKN11,
UYN+13, VHTEG15, ZKW17, dAGNJT12]. QM/Classical [Men15].
QM/MM [AMMK11, DMG10, Exn11, GFRdG11, MOLF11, MG10, SD16a,
SD16b, ST15, SLA12, TIKN11, UYN+13, VHTEG15, ZKW17, dAGNJT12].
QM/MM-ER [TIKN11]. QM/polarizable [Cap16]. QR [BB10, Bou12b].
QR-SCMEH-MO [BB10]. QSR
[KMM+12, MPMMC+11, PH12, XFW+14, ZFW+13]. QSPR
[MPCM+11, SN12, TFA10]. QSPR/QSR [MPMMC+11]. QSTR [PI13].
QTAIM [DP16, MAW+18, Sha11a, VHTEG15, XXJ+16, ZLZ+14].
quadtratic [FYhC11, RSN12]. quadratically [SRK12]. quadratic
[ZST+10]. quadricyclicane [TTD13]. quadruple [MPT11, NZ13].
Quadrupole [MdAdCS12, AC11, BJ12]. quality [OKR12]. Quantal
[SIB+13, SHKS15]. quantification [Gru17, ORJ18, RUS14]. Quantifying
[Mar12, MML11b]. Quantitative
[CJSNLM11, HSN+11, Zha17, MY17, MBTVR12]. quantities [FSST16].
quantization [HKLW13, K111, SD13b]. quantized [Tou11b]. Quantum
[Bal16, BSS16, BL10, BR16, Brá13, Cav13, CKL16, Cho16, COP16, DKZ+10,
DLCB15, DFK16, DLM+11, DC14b, EAK+10b, EML+11, EMEPD15, Ezz10,
FMKJ14, For17b, GbZA10, GGZZ16, HGB08, HS15, Hog13, HB14, Hop15, IFT13, IAK13, IK14, Jen13, JXX+15, KWC10, KYS13, KMK+16, KYH+13b, KUTS10, LB14a, LZZ12, Luz11b, Mak15, Man16, MNE+13, MBTVR12, NTCK13, Nic14, OWD18, ÖEDB11, PH12, PETB18, PKK+16, PSGK17, Puz17, Qu13, RTGS11, Rit11, RMP+14, SAG13, Shi13, SR13, SG14, SBKJ18, SZY17, SSB+12b, Tap15, TFSRM11, UJSJ13, VPN+16, VBJK18, Wag14, WDSL14, WYWL13, WZX+15a, WWX+11, WCM14, WLD+10, XZJ+16, Xu16, YW11b, YZ12, YB11, ZCC13, ZJS13, dFR15a, dFR15b, ASMP15, ABG12, ANC+15, ASK15, BF11, Ban12, Blo15, BGL+16, BHH+13, BT15, BT17. \textit{quantum} [BM16, BBB+12b, Bra10, Brä12, Buc12a, BN11, CM16, CSK12, CSG14, CW13b, Cho15, CYK17, Coo12, CPAT11, CN12, Dau14, DSL15, DPRK12, Dil13, DMBL16, DSFT17, EAH13, FLCHL10, FBO+11, FNT16, FSST16, Gag11, Gan14, GWZ+14a, GB10, GS11, GR10, HR13, HS11a, HITU16, HS11c, HM12, Hor13, IFT14, Ish14, JN13, JMX+15, Kap12, KB12, KCDC15, Kar09, Kar10, Kla16, KCC13, Kit14, Kit15, Kle11, KN15, KK11d, LS17, LSR+13, LCZL15, Lin14, Liu15b, Liu16, LEU+11, Luz11a, Ma14, MC11a, MR12, Mam14, MDC15, MEP15, Mar13, MSC10, MML+16, MPD+10, MQG13, MPL+11, MBBT+12, Mor13, MLDP10, MB12, MGP16, NC11, NKKN15, NS10b, NGS11, NBZG16, Ném14, Nic11, NVPC13+13, NMSR14, NRP+11, NJA+12, Nym14, OPS10, OM13b, OSJ+12, PABSK16, PTH11. \textit{quantum} [PMGMGR12, Pup11b, RP11a, RP11b, RL12, Rei15, RDM+11, RNE10, RN8+10, Rup15a, Rup15b, SOF+10, SBEH11, SKHN13, SC12a, SPSA11, SN15, SK17b, SD13b, She13, SIB+13, SHKS15, SKM11, SGC13, Sjö15, SFY12, SRA+11, SZ15, SCBP17, SPM+15, Tch13, TK16b, TH12, TFA10, Tri14, TB15, UTTh13, UV18, VPFD10, VMR11, VVVB10, Vik11a, VO12, WYM15, WR14b, YÇÖ11, YZ13, YW11a, YS13, YH14a, YW16, YLC17, YLYC18, ZS11, ZX12, ZGSM15, ZH15, ZWSF16, ZZ12, ZWE12, ZRLV10, dHLdS12, dSTH17, vLRRK15, AGNS14, DMS+10, GP13a, ZBK15]. \textbf{Quantum-chemical} [DLM+11, ÖEDB11, Qu13, BF11, DMBL16, DSFT17, MGP16, Ném14, NVPC13+13, SN15, DMS+10]. \textbf{Quantum-classical-aided} [GbZA10]. \textbf{Quantum-classical} [Cho16, Mak15, SPSA11]. \textbf{Quantum-matter} [Tap15]. \textbf{quantum-mechanical} [VPFD10]. \textbf{quantum/classical} [CP11]. \textbf{Quantumness} [CD15]. \textbf{quartet} [HK11, SCZG12, ZCG10]. \textbf{Quartic} [VBC+12b, FT15, dAB17]. \textbf{quartz} [LLM13]. \textbf{Quasi} [XLLZ10, YZ10, BDPT12, Hog13, KUY16, MPM15]. \textbf{Quasi-classical} [XLLZ10, YZ10]. \textbf{quasi-degenerate} [BDPT12]. \textbf{quasi-diabatic} [KUY16]. \textbf{quasi-exact} [Hog13]. \textbf{quasi-stable} [MPM15]. \textbf{quasiparticle} [MS12]. \textbf{qubit} [MR12]. \textbf{quenching} [SAHG11, SAHA12]. \textbf{quest} [GI11d, GI11e, GI11f]. \textbf{questions} [Ng12, VATPR11]. \textbf{quinacridone} [Gao12]. \textbf{quinoline} [MLPT10, MAN15]. \textbf{quinoline-derived} [MAN15]. \textbf{quinolinecarbonitriles} [ZF+13]. \textbf{quinone} [KSAK17]. \textbf{quintuple} [SZS+10, SLZ+11c].
R \cite{DPDR11, DQZF12, GWM11, NBL12, Pan16, CPL15, ESS13, GWM11, LL17, PCR+11, ZSHL14}. R- \cite{PCR+11}. racemase \cite{LZZ12}. radial \cite{IG11, Kha16, RZ17, SPO+11, vLRRK15}. \textit{radiation} \cite{TK16a}. \textit{radiative} \cite{Ber13a, CCM08, SCZG12}. \textit{radical} \cite{BLL+13, BAMA12, BRS10, BCS+12, CWZ+10, GKI2, HWHZ11, IUMVB10, JB11, JAB12, KAR12a, KZA+17, KI12, KZZ13b, LCG12, Les12, LLP+13, LSG+14, LVP12b, MMM12, dMOB12, OKR12, PM17, SSI+10, SPSA11, Sch12a, SB16, SLZ+11b, SLZ+11c, SMS+12, SKM11, SWS+14, WLWL14, XNL+14, YM12, YY18, YSS+10, Zha14, Zha15, ZBK15, ZLWL16, ZJC+13}. Radicals \cite{TWHZ14, lAyL14, Buc12b, CGIAI12, DI11, DFK16, HXX15, KK14a, LCL+11, LVP12b, NP18, RLW+13, TIN13, TCA10, YM13, YL10}. radii \cite{GI10, SV11, TMC+13}. \textit{radius} \cite{Bar11}. \textit{Radu} \cite{Tou13}. Ramachandran \cite{MAW+18}. \textit{Raman} \cite{CK13, VV13, C¸AS13, KV11, LMZY15, PM12, SSI+10, SK14, SPSA11, Sch12a, SB16, SLZ+11b, SLZ+11c, SMS+12, SKM11, SWS+14, WLWL14, XNL+14, YM12, YY18, YSS+10, Zha14, Zha15, ZBK15, ZLWL16, ZJC+13}. Radar \cite{TK16a}. \textit{Rapid} \cite{AA15, NE11}. \textit{rare} \cite{BAP12, BGL+16, DLG12, JEA13, MURR13, YJ17}. Rashba \cite{SBD+16}. Ratchet \cite{BEZP10b}. \textit{Rate} \cite{WZHZ13, AFM+10, Buc12a, CAAI12, CGIAI12, FLCHL10, FBM+10, MVC13, NZLG15, dMOB12, ZLWL16, ZXY13, SSP14}. rates \cite{AC11, CCM08, RFEGPP+16, YK13}. Rational \cite{LLZ+14, WR14b}. \textit{rationale} \cite{JWJ+12}. \textit{rationalization} \cite{ZXY13}. ratios \cite{MOY13, TSL11}. }
ZXY13, ZSS\textsuperscript{13}, ZJC\textsuperscript{13}, Zil14, dHLdS12]. reaction-field [SHMR11].

Reactions [KKH\textsuperscript{13}, LLM13, MNE\textsuperscript{13}, OD12, TIN13, TM13, ACMRN10, BR510, BS14, Buc11b, CdAFS\textsuperscript{12}, CM12, Chr10, CJGTL12, DWJJ11, DAA16, DFK16, EMED\textsuperscript{12}, EMEPD15, FRNM12, FDMR11, GGZZ16, HDC\textsuperscript{11}, HLM11, HB14, Hop15, HXX15, HCL13, Kan11, KZZ13b, KMM16, LW11, LLF17, LGW11, LSG\textsuperscript{14}, MAP\textsuperscript{10}, NAK\textsuperscript{17}, dMOB12, RLW\textsuperscript{13}, Sch12a, SHS\textsuperscript{13}, SWS\textsuperscript{14}, TFZ\textsuperscript{15}, Var14, WLG\textsuperscript{11}, WLWT12, WZH13, WLWL14, XLLZ10, YSS\textsuperscript{10}, ZGSM15, ZXY13, ZQXP17].

reactivated [MG10]. reactive [Cho15, dDGNB10, RL12, Ser11b].

Reactivities [YM13, LLZZ10, MDNDO\textsuperscript{16}]. Reactivity [KSC15, OPFI11, PMH\textsuperscript{16}, TWHZ14, TV13, BVRM10, Cha11, DVC14, DNCKCS\textsuperscript{12}, ESBVJY12, GGP13, Hog13, JWJ\textsuperscript{12}, KP10, KO14, MMM12, MUNZVR12, MAP\textsuperscript{10}, MBA\textsuperscript{13}, MBBT\textsuperscript{12}, MCRS16, NAK\textsuperscript{17}, NE11, NZAVR10, RGS\textsuperscript{13}, RBLZ15, Ser11a, SC10b, WJ11, YSK\textsuperscript{12}, RdA11].

reagent [BPT12, LWWZ13]. Real [GKT\textsuperscript{12}, HR13, Fin14a, FNIT16, GI11b, GI11c, PI16, RLER13b, SHKS15]. Real-time [HR13, FNIT16, PI16, SHKS15]. realistic [SPSA11]. realization [PM12]. really [SMR14]. rearrangement [KMM\textsuperscript{12}, CRSB12, CSVCB12, MSY\textsuperscript{12}, SSP\textsuperscript{17a}, SK11, WTH\textsuperscript{11}]. receptors [PRG\textsuperscript{10}]. recipe [STM18]. recognition [AGRI\textsuperscript{12}, JNY17, PvS10]. Recognizing [Cav17].

recombination [BMF13, dMOB12]. reconstructed [dLdOdAD12]. Reconstructing [YS13]. reconstruction [GD11]. reconverge [SWS\textsuperscript{14}]. rectangular [Lun13a, Lun13b, MPD\textsuperscript{15}, Tou13, YMY\textsuperscript{13}]. Recursion [LWY13]. recursive [SGH10]. red [FSBA12, Kry10, MRÅ11]. red- [Kry10]. Redox [MLY\textsuperscript{16}, AGJ12, BBA\textsuperscript{16}, ESS13, KB13, KRK\textsuperscript{17}, LCH14, VLG12]. reduced [ABLT11, CM15, KK13, Lat13, MPE11, Per18, dCGAMV12].

reductase [SDM12, SLS\textsuperscript{10}, TSKN12]. reduction [KGK13, QCW\textsuperscript{12}, WTW\textsuperscript{11}, YHL\textsuperscript{13}]. reevaluation [GI14]. reference [NS13, NF11, SBKJ18]. refined [SYK\textsuperscript{12}]. reflecting [AA11]. reformulation [Lev10]. refractive [SHMR11]. Regina [HS15]. regio [CM12, GHCMCMQ17]. regio- [CM12]. regio-selectivity [GHCMCMQ17]. region [EMED\textsuperscript{12}, KYS13, OVT\textsuperscript{16}]. regional [NGS11]. regions [LdB12]. regioselective [Iku17, LKZ\textsuperscript{16}]. regioselectivity [DPDR11, DMWY11, NAK\textsuperscript{17}, Zha15]. regression [VSL\textsuperscript{15}]. regular [PR10a, Pa10]. rehybridization [Sch15]. REIN [MRS15]. Reinvestigation [NHJ11]. relafen [YINM13]. related [Buc12b, HNH\textsuperscript{12}, Luz13, RLW\textsuperscript{13}, SSI\textsuperscript{10}, TD11, UMS13, VLG12, WLWL14]. Relation [PM16, KM12c]. relationships [AE12, DB13a, GZSMFN16, LWY13, RS13]. Relationship [CZJZ12, DNCKCS\textsuperscript{12}, GXZ\textsuperscript{14}, Gra08, Gra11, LBdV16, MY17, RGST12]. Relationships [NBI\textsuperscript{10}, CJSNLM11, EKN10]. Related
relatives [Fin14a], relativistic
[Fri12, Liu14, CSG14, DAC12, FSST16, MPTZ13, MZST16, NSN17, NNSN17, RTT10, SN15, SS12, ZKKR11, ZQXP17]. relaxation
[BMF+14, EBR11, FLK+12, Krt17, Ng12, RMJ11, SIM14, YT14, ZP16].
relaxed [RS10]. release [SYK+12]. Relevance [Eng16]. relevant
[ASHF13, KSD10, MPTR12, Wag14]. reliable
[BMF+14, EBR11, FKL+12, Kit17, Ng12, RMJ11, SIM14, YT14, ZP16]. relaxed
[RSL10]. remediation [RdPW+12]. representations [DJ95, FLvLA15, RSL10, DJ12]. representative
[SKHN13, TFF+15, WLW14]. Review
[Ban12, Bra12, CD15, CSG14, CLXD15, DVC14, DSL15, DC14b, Dui15, FZ14, For17b, HJ13, HFGC14, IN15, LJ13, Lin14, Mai14, MC14, Nym14, PM16, RP13, SMMT13, SBD+16, Tay12, Val13, WR14b, WCM14, ZP16, dGR14, Beh15, LFF+10, Li11, Liu12, Liu15b, MWH15, Mor13, RF10, Sch0a, YZ13, YKM+15, Kry11a, Mas11, Mue12, Liu16]. Reviewers [Cav17]. Reviews
[AB16a, AGNS14, AMAM18, Bae16, BW18, BC15, Beh15, BBB16, BM16, BBA+16, BS16, BW13b, Cap16, COCF+14, CM15, CSS16, CML16, D'y16, FP16, GZ16, HK15, Hop15, HX15, JW18, Jia15, KC13, KKL+16, Laz14, Li15, LGZ15, LSP+16, LMZ15, Liu15a, Liu15b, LKd+16,
MHO$^{+15}$, MMG15, MDC15, MWH15, MW16, MMÅ13, Mos14, MZST16, NBZG16, OWD18, PDR$^{+14}$, Ped16, PSMD16, Per18, PETB18, PI16, Rup15b, SFC16, Sch13, SB16, SHKS15, SG14, Sjö15, SCB$^{+14}$, SZ15, SPM$^{+15}$, TTD13, T$\text{SV}_L^{+16}$, Tch16, TK16b, TB15, Tsn15, Var14, WZX15b, YZ13, YKM$^{+15}$, YZW15b, YH14b, YHLC15, ZF15, ZPZ15, ZBK15, ZB18, vL13, SGJ10].

revisited [DVDBM11, OPC17]. Revisiting [GGP13, MJ16a, NS10b, VVJ15].

Rg [BPG$^{+10}$]. Rh [BLRdA$^{+10}$, MMRRA10, PRPU$^{+13}$, RYW$^{+15}$, SBB16].

Rh-doped [RYW$^{+15}$]. rhenium [YZW$^{+15a}$]. rhodanine [EAK$^{+10b}$].

rhodium [DSH$^{+13}$, LYR$^{+17}$, MMRRA10, WML10, ZZC15].


ribbon [WWL$^{+11}$]. ribbons [SPD$^{+18}$]. ribose [ZWK17]. rice [WH$^{+13}$].

rich [TCSD12]. Ricotta [HS15]. ridge [VSL$^{+15}$]. rigged [IFT13].

right [KBJ17]. rigorous [Mak15, vL13].

Ring [BR08, RB08, AKR12, CLXZ12, DLLA10, GZ14, KMS$^{+11}$, KUTS10, LWJL10, LLLB13, MSK11, NHG$^{+12}$, QB15, Sat11a, WDSL14, WCY$^{+10}$, Yami10, YZ12, YT14, Zha14, BR12a, RB11a]. ring-polymer [YT14]. rings [ABTW14, BR08, BR12a, BBKO16, RB08, RB11a, RNV$^{+12}$, TKS11, VC13, WvRSW$^{+11}$, WWD$^{+15}$].

rippling [MFM18]. RISM [KSS12].

Ritz [MB12, SBM16].

Robust [AAAM12]. robustness [Fin14a]. roentgenium [DR18].

Role [BR12b, CM16, HSYM11, PCML08, AM13b, BLWJ17, CG12, CHSO13, DS11, EMK14, EMSB15, FNBK17, GBZA10, GLOGM$^{+11}$, JNY17, KGVI11, KKG12, LSR$^{+10a}$, LSR$^{+11}$, LQ13, MAW$^{+18}$, Msov13, Per10a, PWH$^{+12}$, RMJ11, SFL$^{+10}$, SHL$^{+13}$, SFP14, SCI11, SC18, Var14, WCGD12, ZQW$^{+17}$, ZWE12, dAVdM17, WLW$^{+12}$, MB12]. roles [JLG$^{+12}$]. room [TD11].

Roos [Pyy11, SA11b, Sha11b, SL11].

Rosa [dGR14]. Rosen [PSGK17, Tou11a, ZHF12]. rosiglitazone [HSS$^{+11}$]. rotamer [CodF$^{+11}$].

rotamers [HNN$^{+12}$]. rotary [OWD18]. rotating [HRT12, KBG17, Sta10].

rotation [AO12b, CPL15, DDF$^{+12}$, HK11, HRT12, KBG17, QD10, Sut12].

rotation-vibration [HRT12, QD10]. rotational [AEÖ12, CCBR$^{+12}$, DCR10, Puz17, RMJ11, SPO$^{+11}$, VLM$^{+10}$]. rotations [JdOS16, KMS$^{+11}$]. rotovibrational [PBB15]. route [BMF13, HGB08, SRS$^{+17}$]. routes [VPGC12].

Rovibrational [LPL17, AM12, FT15, VLF12]. rovibrationally [Dau16]. row [BZBZ13, KWC11, MKM11, ZFC$^{+17}$]. RPA [LZ10]. RKKM [DS12, STL12].


RuCl [CCL$^{+10}$].

rule [DMWY11, JLI12a, KT12a, MHT$^{+08}$, SD13b, XWC10, YLZ$^{+17}$, KK11b].

Rung [Jan13]. Russian [Tch16]. ruthenium [CWB$^{+13}$, LYL$^{+12}$, SLS$^{+15}$, LGS$^{+16}$].

rutile [EFO11, GP13a, HCL13, ZLWY13]. Rydberg
Rydberg-like [DTPC17].

second-row [ZFC^{+}17]. secondary [CLL^{+}11, LLLT^{12}, PCML^{08}]. sections [CK^{13}, MKG^{+}11, NA^{14}, VV^{12}, VV^{13}]. SEDD [KSS^{12}]. segment [MYZ^{+}10]. segregation [GE^{12}a]. SeHCl [MZLM^{17}]. select [AC^{11}, VRM^{11}]. selected [CCA^{+}12, EMED^{+}12, EMEPD^{15}, KM^{12a}, Kin^{13}, MMWA^{11}, MLB^{+}12, Sic^{16}]. selection [YKN^{13}]. Selective [SSP^{+}17a, SLS^{+}15]. Selectivity [IUMVB^{10}, GHCMCMQ^{17}, MAP^{+}10, MPE^{11}, TFA^{10}, VBJK^{18}, ZPW^{16}]. seledine [MA^{11b}]. selenium [DLLA^{10}, ESDO^{16}]. selenium-containing [DLLA^{10}]. selenocyanate [KMS^{+}11]. selenopeptides [Dum^{12}]. selenylsulfide [Dum^{12}]. self [Chr^{10}, ISN^{13}, Bra^{11a}, FFF^{10}, Fin^{15}, GRD^{11}, KKH^{+}13, LYW^{11}, QTCL^{10}, RAK^{10}, SIM^{14}, SY^{10}, SHMR^{11}, VFSC^{17}, WDJ^{+}17, ZZW^{11}]. self-assembled [KKH^{+}13, QTCL^{10}]. self-assembly [FFF^{10}, LYW^{11}, VFSC^{17}]. self-consistent [ISN^{13}, Fin^{15}, SY^{10}, SHMR^{11}, WDJ^{+}17]. self-consistent-field [GRD^{11}]. self-energy [SIM^{14}]. Self-organization [Chr^{10}, Bra^{11a}, RAK^{10}]. self-biorthogonal [BVP^{14}]. semi-core-valence [Eng^{16}]. semi-empirical [Hat^{13}]. semi-infinite [MFLK^{11}]. Semi-local [RPV^{10}]. semicarbazone [YW^{11}]. semicircles [LQZZ^{12}]. semiclassical [CPAT^{11}]. semiconductors [BWE^{16}, Eng^{16}, HKZZ^{15}, YHL^{+}13]. semi-direct [Tri^{14}]. semi-empirical [Bou^{11}, GI^{10}, BO^{11}, KD^{12}, MSVMC^{10}, RS^{11b}, SM^{14a}, WKE^{17}]. Semilocal [PSMD^{16}, SFC^{16}]. Semiquantum [OHDA^{13}]. semirandom [Pog^{12}]. semiregular [Bib^{13}]. Sensing [NEEV^{15}, Man^{16}, MBSAG^{16a}, MBSAG^{16b}]. sensitive [CC^{11a}, MP^{12}, PJ^{10}]. sensitivity [Bon^{17}, ORJ^{18}, YZ^{13}]. sensitized [AGJ^{12}, BDG^{17}, FM^{16}, clqFt^{W^{+}14}, MY^{17}, MANP^{17}, PMA^{12}, QJ^{13}, SSS^{15}, WVB^{+}14, Zha^{17}]. sensitizers [CWB^{+}13, LGS^{+}16, SSS^{15}]. sensor [HNBG^{15}]. sensors [FBU^{+}11]. SeO [ZLY^{+}14]. Separation [Nal^{13}, BLKB^{11}, MPD^{+}15, PETB^{18}, SSP^{+}17a]. separations [PWP^{13}]. Sequence [NMS^{+}10, CLC^{10}, HW^{12}, YSW^{11}]. Sequence-dependent [NMS^{+}10]. sequences [Gar^{08}, GIFW^{11}, HXD^{16}, KA^{11}, Lad^{14}, LQZZ^{12}, LLZa^{14}, XTLa^{13}, XTLa^{14}]. sequencing [Che^{13}]. Sequential [MBMK^{12}, KB^{12}, MFB^{11}]. Ser [ScBsR^{+}10, TK^{16a}]. Ser-His-Glu [TK^{16a}]. series [BDPT^{12}, CWS^{15}, CKY^{17}, DSRGD^{12}, DB^{13a}, MBBT^{+}12, MSR^{+}11, SUL^{+}11, SK^{12b}, SZL^{+}14, XFW^{+}14, YZL^{+}10, ZQ^{13}, vLRRK^{15}]. serine [CLMY^{12}]. serine- [CLMY^{12}]. serotonin [CSVC^{12}, CSSK^{+}12]. Serrano [Mer^{11}]. Serrano-Andrés [Mer^{11}]. SERS [TSBS^{12}]. serve [Fin^{14b}]. serving [DSRGD^{12}]. set [Ali^{14}, BVCAP^{12}, Chua^{12}, DCZ^{17}, Fuh^{12}, HZG^{12}, JA^{12}, JH^{15}, KRC^{+}16, KYS^{13}, LV^{12}, LWL^{+}12, MG^{12}, ND^{+}12, PWP^{13}, Rud^{12}, SKTH^{15}, SZ^{+}10, SLZ^{+}11c, SLZ^{11a}, SL^{+}11, TP^{MB}^{12}, TWR^{15}, VPA^{11}, VSS^{11}, YFY^{17}]. sets [ANC^{+}15, ABA^{11}, BL^{16}, GS^{10}, Hl^{13}, MSNP^{18}, PCD^{14}, RLR^{14}].
RVO$^{+14}$, UV18, VRO$^{+12}$, Zak13, ZF15]. **seven**
[BR08, BR12a, RB08, RB11a, RN12]. **Seventh** [NYA$^{+13}$. **Several**
[Tch16, MMM$^{+12}$, SLSZ13, XYS10, YIY$^{+13}$]. **sextet** [AM12]. **sextuple**
[SLZ$^{+11a}$]. **SGSA** [SOF$^{+10}$]. **SH** [BDF$^{+16}$, CdAFS$^{+12}$, dSNBG08].
shallow [CN12, Fuk12]. **Sham** [BW18, Bar11, Gan14, KdSM$^{+10}$]. **Shannon**
[JZZH17, Nag15, Sit15, SDL$^{+15}$. **Shape**
[NMV$^{+14}$, BXR$^{+13}$, BVP13, KP11, LKN13, SSAM13, XWCY11]. **shape-**
[LKN13]. **shaped** [BN11, KKH$^{+13}$]. **shapes** [IROW$^{10}$]. **sharing** [BBKO16].
**SHCl** [MZLM17]. **sheet** [SJW13]. **shell**
[CP16, Fin14a, Fin15, GBS17, GXZ$^{+14}$, JEA13, KK13, MSRn$^{+11}$, NSN17,
NNSN17, STM18, SDY16, YMY$^{+13}$, dSdS13b, dG14]. **shells**
[GHP11, Puh11]. **shielding** [Cyb11, MGK$^{+11}$, NB17, RRK16, SS12]. **shift**
[Bou11, Bou12a, LCB10, MFB11, Rit12a, Rit12b, SCB$^{+14}$, SK10, TKSK17],
shifted [AHHN16, Kry10, Roy14]. **shifting** [dOR10]. **shifts**
[CRSB12, CFGC11, FBD$^{+13}$, Tap15]. **SHN** [NRP$^{+11}$, SS11]. **short**
[Dum12, GST11, NWQX11, SB16, WWL$^{+11}$. **short-living** [SB16].
**short-loop** [Dum12]. **shortcomings** [MGN14]. **should** [She13]. **shuttle**
[FDMR11]. **SHX** [EMS15]. **Si** [GLF$^{+12}$, JL12a, MGD11, TW10, TFB11,
UKF$^{+11}$, VPFD10, CN12, ENV15, LKN13, LBY$^{+14}$, LLLL13, MCP10,
MBA$^{+13}$, MSV110, OD16, PWL$^{+10}$, WLWL14, ZCX$^{+16}$]. **Si-**
[ZCX$^{+16}$]. **Si-doped** [ENV15]. **SiC** [XL11]. **SiC** [TCCI10]. **SiCH** [FT15]. **SiC** [SD16a].
**side** [DSOC$^{+13}$, MPE11, NHG$^{+12}$]. **side-chain** [DSOC$^{+13}$]. **SiF**
[KMM16, KMM16, SLS$^{+12}$. **Si-Ge** [LLL13]. **Sigma** [DAC11]. **signal**
[QZH13]. **signature** [GDM$^{+10}$]. **signatures**
[BR08, BR12a, RB08, RB11a, ZR13]. **signed** [SK17b]. **Significance**
[Chu12, ELC08, Kut10]. **Si** [HCL13, RLW$^{+13}$]. **silapolyacetylenic** [TYL10].
**silica** [CRSB12, SFNC$^{+18}$]. **silicate** [Ped16]. **silico** [DAA16, ST15]. **Silicon**
[Cza18, AMK10, CSK12, JLS13, KAG08, KMM16, LRK10, LHL$^{+15}$,
MSK11, NEEV15, RK14, RKM12]. **silasesquioxanes** [TD17]. **Silva**
[COP16, HS15]. **silver** [AMK10, Boc12, SS18, YJ17]. **silylene**
[LCH$^{+11}$, LXL11]. **similar** [Pup11a]. **similarities** [BB16, MK10a].
**similarity** [ART08, Luz11b, MBT12, MBBT$^{+12}$, Sat11b]. **simple**
[BM16, DCR10, Fin15, FB17, KV11, Lev10, LPM$^{+11}$, MA12, MT10, SAS$^{+12}$,
SGL$^{+16}$, SGK12, STM18, TLC$^{+17}$, TC12, VSL$^{+15}$, YZZ16, ZT13, ZDF13].
**Simplification** [CFOCR10]. **Simplified** [GZF14, GZSMFN16]. **simulant**
[HYZ13]. **simulate** [SK12]. **Simulated**
[TCG17, VVS$^{+18}$, AM13a, Eil14, JPP$^{+11}$, MOE$^{+11}$, VNN$^{+16}$. **Simulating**
[DBM15, MRS15]. **Simulation**
[LP6$^{+11}$, CwCW$^{+11}$, CSK12, CS17, CTDOLA10, DKZ$^{+10}$, DGR$^{+16}$,
DLZ11, FF10, Fm17, FTN16, Hog13, IFT13, IFT14, KST12, LCT14, LL17,
Mas14, MPD$^{+10}$, MPZWD10, MG12, NKK15, Net12, NDM$^{+12}$, PP10,
PMH$^{+16}$, SLS$^{+10}$, Tan13, UTT13, YAF$^{+15}$, YT14, YIN13, ZWSF16].
**Simulations** [Hor13, MSH13, Mar13, OHDA13, SIB$^{+13}$, SHS$^{+13}$, UYN$^{+13}$,
UTT13, YK13, ÁF12, ATS15, BMF$^{+14}$, BM10, CLKD15, GVPCK10,
solutions [AEÖ12, EI11, HYZS12, LDZG16, LEU+11, PS10a, PVS11, PVS12, PT13, PGMGRM15, RMLPGGH16, SMV11, TIKN11, ZLJ11, ZHF12, ZPFZ15].

Solvable [GMGRMP12, Kub12, PGGRMP10, PMGMGR12].

Solvated [CLMY12, LCCH11].

Solvation [GLPA10, MSK12, BH10a, JCC10, Li15, Owe17, PCR11, RFN12, SL10].

Solvatochromic [LCB10, MFB11].

Solvatochromism [Men15, MRÅ11].

Solvatofluorochromism [FSBA12].

solve [Blo15, CRA+11, Ign11, Ign12, Kri13].

solved [SW10].

Solvent [EKD12, RdA11, RMTG11, dAvM17, BS11, Cap16, CYLL11, CS17, DLO16, DFF+13, GZF13, HFL+17, IGKM11, IK14, JN13, KI15, LWL+12, LLC+11, LWJL10, LDW+11, LLZ+12, MG12, MKHM11, QHS11, SN12, TC10, WLD+10, XX12, XWC11b].

solvents [COCF+14, HFL+17, KP10].

Some [Brä11b, Jou13, Luz12, SW10, Sut12, VATPR11, ZYL+14, AF16, AMAM18, BCGC12, DCR10, EA+10b, EA+10a, EI11, For12, GCDNGS12, GB10, GI11b, GI11c, HS11b, KCC13, Kin13, MANP17, MAP+10, PL11, Pie12, Roy13, SGL+16, Tch16, TCA10, VO11, XHZXXZ10, ZCC11, ZLZ+14, ZZC12, Sic16].

SOS [RNC14].

SOS/QM/MM [RNC14].

soundness [Sha11a].

source [GCK+17, Hor13, QSX+15, RAMB18].

sources [LTdSJ+10].

sp [She13, MCK17].

space [BPV13, BGBV12, CDT12, Fin14a, GRD11, HN12, KPH+12, MSNP18, MFLK11, MQA17, NaN12, NaN13, PC16, RW12, SKT15, SBL11, VM1R11, WWL17, vL13].

spaces [LYW11].

spacetime [RW12].

spanning [Bib13].

sparkle [FS11].

spatial [ABP13, Pit12, SR12].

spatially [GZF14].

Special [´AIGVZW12, For17a, LV16, NYA+13, NT15, OS12b, Rei15, Rup15a].

speciation [HFL+17].

species [GS11, HJRO13, MG1D1, SS+10, SM14b, SM14c, SM14d, SM16, YHLC15, dHLdS12].

specific [LZD+11, MMS+12, Nic11].

specificity [PS10a].

Spectra [MLY+16, AEKGZ12, AFC+10, AFV12, AEM+12, Ban12, BBB+12a, BS11, Ber13b, BBa16, BBAL12, CP10, CFP+10, CS17, CML+16, CLMY12, DSH+13, Eli14, FBO+11, For12, GIO12, ILBS10, IHH10, JPPA10, JPP+11, KV11, KBMM10, LYY11, LWL+12, LMZY15, LLP17, MC11a, MPJ12, MSK11, MAA13, Mor13, NBI+10, OVT+16, ORJ18, PR10a, PCR+11, PJ10, RNC+14, SBAT16, SB10a, SPO+11, SZZZ11, TZ11, TFSRM11, TT10, TG13, VPPD10, VVS+18, VSN+11, Zen11, ZQCJ10, ZWLC12, ZLE17, ZSZ14, ZQXP17, dARA13].

Spectral [LLH15, Mys12, CdLdSC18, FBU+11, KP12, LYR+17, SGZ13].

spectral-luminescent [KP12].

Spectral/structural [LLH15].

Spectroscopic [BH10b, Jac12, Mag14, NC11, NVPCT+13, SXS+10, SLZ+11c, SLZ+11a, SLS+11, SX+12, SLS+12, WFS13, BD12, CHM+14, CWB+13, CJOOW11, DAE+12, GFB12a, KSS16, LJSS12, LZZ+17, MG12,
MPTZ13, QHS11, RNdA\textsuperscript{+}10, Sch10b, SLSZ13, SWS12, Tas14, VLG12, VLFG12, VBO\textsuperscript{+}15, WX\textsuperscript{+}11, YZL\textsuperscript{+}10, YZL\textsuperscript{+}11, ZLLS10, ZR13, dSdSPG11.

Spectroscopies [KKT13, MOY13, McC13a, OA13]. spectroscopy [Beri13a, BDR12, For17b, GFB12b, LdBF\textsuperscript{+}12, Mas10, MML11b, ORJ18, Ped16, Puz17, SA11b, UTTu13, YJ17, ZPZ15, RdA11]. spectrum [AA11, BS16, BBB\textsuperscript{+}12b, Bou12b, CWF11, CRSB12, DHZS11, DWGX12, HHCA10, HRT12, HMH\textsuperscript{+}13, HYH\textsuperscript{+}10, JCC10, KBG17, NDM\textsuperscript{+}12, QD10, RS12a, SBKJ18, WWC17, Zha17]. Speculation [KRH13]. spent [HB14]. spermine [SGB11]. Spherical [Kit15, PML\textsuperscript{+}11, Roy15, CH17, CN12, Nik11, OHDA13, RLER13b, Roy16]. Spherical-harmonics [Kit15]. Spherical-harmonics [JZZH17, Nag16b]. spheroconal [MFLK10]. spherically [JZZH17, Nag16b]. spheroidal [OPC17]. Spin [Kle11, Luz11a, MLK17, SAHG11, SAHA12, Swa13, YY1\textsuperscript{+}12, ATL\textsuperscript{+}14, Ber13b, Bla15, Bra10, CFGC11, CSP\textsuperscript{+}10, CDT12, DS11, DM16, FSST16, GXZ\textsuperscript{+}14, GFRdG11, Joh17, Kap12, KK14a, KSN\textsuperscript{+}10, KYH\textsuperscript{+}13b, LVdSdM14, LWL\textsuperscript{+}12, Luz12, MR12, MPRB\textsuperscript{+}10, Mos14, MPRB\textsuperscript{+}10, MC18, MC18, NNS17, OS10b, Qu13, RS12a, RLZ12, SR12, SRSZ16, SSP\textsuperscript{+}17b, SBD\textsuperscript{+}16, T\textsuperscript{+}10, TD11, WH12, Yur13, Yur15, ZSQ\textsuperscript{+}10]. spin-dependent [DS11, NNS17, NNS17]. Spin-free [Kle11, Luz11a, Luz12]. Spin-Hamiltonian [TD11]. Spin-orbit [MLK17, MC18, RS12a]. spin-projection [KYH\textsuperscript{+}13b]. spin-restricted [KYH\textsuperscript{+}13b]. spin-spin [CFGC11]. spinless [NF11]. spiro [LLLB13]. spiro-heterocyclic [LLLB13]. spiroborate [QCW\textsuperscript{+}12, WTZ\textsuperscript{+}11]. spiroiminodihydantoin [SM13]. spline [HZS14]. split [GRD11]. split-graph [GRD11]. splitting [GWM11, HYH\textsuperscript{+}10, SYK\textsuperscript{+}12, SSK\textsuperscript{+}12, Tan13, YY1\textsuperscript{+}12]. Spontaneous [CCM08]. spread [BEM12]. square [LGHL11]. squaric [DLM\textsuperscript{+}11]. squeezed [PSGK17]. SR [MC18, MPD\textsuperscript{+}15, MGP16, Oni10]. Sr-doped [Oni10]. SrBi [HLMO11]. Sr [ZFW\textsuperscript{+}13]. SrH [HMI\textsuperscript{+}15]. SrTiO [OH13, WCL\textsuperscript{+}17, OH12]. SS [SZZ\textsuperscript{+}12]. SSH [DTF15]. stabilities [AF16, MS17, SF2W, SU1\textsubscript{+}11, SM14c, ZYL\textsuperscript{+}13, dAVdM17]. Stability [GV11, KZA\textsuperscript{+}17, Kry11b, MC12, TCL\textsuperscript{+}17, USL\textsuperscript{+}13, Boe12, CWSZ13, DVC14, FBRBR12, GB13, GAMM10, GWJ12, Ire12, KK11b, Kry12b, LGHL11, LCZ15, LGs\textsuperscript{+}16, MNV\textsuperscript{+}17, MC17, MCARL11, MJ14, MM10, MS14b, MHHP\textsuperscript{+}17, Ng12, NRI15, ONK\textsuperscript{+}13, Owe17, Pat15, RN12, SFNC\textsuperscript{+}18, WJL\textsuperscript{+}11, WCS\textsuperscript{+}13, WJL\textsuperscript{+}10, YZ13, ZBBB17, GCD13]. Stabilization [YZZ15, JdL08, MK11, OKR12, SBMM11, YD17]. stabilizer [OKK10]. stabilizing [MK12, PCML08]. Stable [Sat11b, BMF13, MPM15, MAN15, PAPCMM\textsuperscript{+}16, ZCG\textsuperscript{+}16]. stacked [NMS\textsuperscript{+}10]. stacking [ACF\textsuperscript{+}11, DB15, FSB16, KdPNNS16, LB18, ZS12]. stacks [FV11]. stage [Kap12, SZ15]. stages [LJ16]. Stagnation [PL11]. standard [KGK13, PJP08, Tug13]. State [HXX15, NBZG16, Nic11, ACF\textsuperscript{+}11, Ang10, BPVDB11, BMF13, Bon17, Caol7, CMCN11, Cha11, CJOOW11, DGA\textsuperscript{+}13, EMEPD15, FRGC10, FSBA12, GSA11, GWZ\textsuperscript{+}14a, GWHH17, Ghu13, GLOGM\textsuperscript{+}11, HM12,
YLWrL12, ZHI17, ART08, CWB+13, DMBL16, EPS+16, GMP+11, IAK13, KG17, LHI15, LZ10, MB14, MSK+12, MA11a, MHKM11, MW15, ORJ18, PK13b, RJY+10, RNDA+10, TOSN12, TBST10, TFB11, VLG12, WHT+11, WLL+13, WWD+15, YD17, ZWLC12, structurally [DC14b].

Structure [AKHS13, Ber13a, BMBD10, Boc17, CM15, FBRBR12, KSG+12, KKT13, LYW11, MMMM12, MCARL11, MOY13, MCI13a, MTS15, OA13, Owe17, PAKA15, SIT+12, TBA13, Wu11, YSK+12, AB16b, AEKGZ12, AOI2a, Ale13, ATS15, BZBZ13, BL10, BG11b, BG11c, Bou11, BOu12a, BOu12b, BA13, CLL+11, CZZ12, CWL+13, CJSNM11, Cas15, CSVCB12, CJOOW11, DCBB11, DIOG12, DVC14, DDY12, DMBJ15, DD17, DGA+13, DZO12b, DSH+13, Dy16, FLvLA15, FBO+11, Fin14a, Fin15, FBU+11, GBS17, GSZ10, GZ14, GP13b, GEL18, HMI+15, HLMO11, HJ13, IGMMK11, IK18, JWG+12, KS11, KK11b, KK11c, KRR+17, KJ15, KJ16a, KJ16b, KS10, Kl+11, KSB11, KAOB11, KP13, KO12, LW1+11, LLLT12, LZZ+13, Ly14, Ma14, MC11a, MY17, MSG16, MSH13, MPD+15, May14, MBA+13, MPWD10, MCL11, MS14b, MK11, MLB+10, MJ11], structure [MCRS16, NDM+12, PCML08, PT13, PMMGL+11, Puz10, QTCL10, RFN+12, RS12b, RKM12, RGST12, RMTG11, RUS14, RMY+13, SMK+12, SC12b, SB16, SRS+17, ST011, ScB1R+10, SSW16, SBK1J8, TD11, TSH17, TG13, TPJ+12, Var14, VLM+10, Ven12, VSS+11, VBO+15, WCS+13, WSV10, Yak11, YLW+13, YRN+11, Zha10, dOLdL13, GFB12b, GGD12, NA12].

Structure-dependence [KSG+12], structure-property [RGST12].

structure-stability [DVC14].

Structuring [KRG+13]. studied [AMMK11, BL10, CK17, DCHC11, FBO+11, TTM16, ZL10, dSDS13b].

Studies [Roy13, ACF+11, AMK10, BD12, Buc11b, CCA+12, ÇAS13, CY1L11, CTW12, CWB+13, CSVCB12, CSSK+12, DSWL11, DB15, EAK+10a, EA1+10a, EI11, For12, GGD12, GKT+12, HT10, HNAG15, Hop15, HWL16, JL12b, KL+12, KD12, KA13, KSY+11, KAOB11, Le12, LWL+12, LS+13, LBY+14, LGZ15, LWJ10, LK1111, MANP17, MLPT10, MAP+10, MMM+12, NTCK13, ONBP11, OEDB11, BPM10, PTD+12, PETB18, PACCMM+16, RJV+10, RJA+10, RGT11, RNA+10, Ril10, Riv11, RGS+13, RGR12, Roy14, SMK+12, SD16a, SC12a, SJZ12, SIS+08, SK12b, SZ1, SSB+12b, TIKN11, TOSN12, TYN13, TAY+11, Tan12, TIN13, TX10, THSR13, UJSJ13, WZX11, WTH+11, Wan13, WZM+13, WYWL13, WHMI14, XFW+14, YY1+10, YY+15a, YB11, ZL11, ZZ10, ZYY+11,
ZQJW13, ZLWY13, ZLZ14, ZSZ14, dAGNJT12, YWY12]. **Study**
[Bar11, CH17, IFT13, IFT14, SGL16, ZCP11, AFC10, IAYL14, AM12, AASU17, ATMI17, AKC10, ASW13, ASD14, AMAC12, BMK14, BD14, BF11, BGC12, BFD16, Bas11, BAMA12, BL12, BS11, BEM11, BZB13, Ber13a, BL11, BLR13, BS14, BZZ15, BDG17, BMF13, Bon17, BDR12, BCF11, BPM12, BL12, BJ17, BjdMAV12, Buc10, BO11, BVRM10, BCS12, BB16, BSV12, BSK11, CRB12, CMR13, CAZ11, CLQZ12, CCL13, Cao17, CPL15, CPF12, CCBR12, CHM14, CG12, CW16, CM12, CCL10, CCH12, CSS13, CWW16, CZL17, CLY12, CS13, CWS15, CK13, CFGC11, CGIAI12, CAPL12, CPAT11, CJOOW11, CD12, CS18, DW12, DCP11, DIO12, DM12, DAR11, DKS11, D13, DCDD10, DSRG12, DPK12, DPD11, DTEM11, DZ11, DDo11, DW12, DQ12, DSH13, DCR10, DSFT17, DFD13, EG10, ESDO16, EAH13, EFO11, EO11, EB11, EA12, ENV15, ES17, ESBJ12, FQ11, FFF10, FO10, FM16, FTH11, FRR12, FDR10, Fin14a, FT15, FPPGMB12, FBU11, Gab11, GBS17, GWM11, Gao12, GLF12, GGJD13, GZW16, GHG12, GKI12, GFB12b, GMP16, GS11, GLOGM11, GHCMCMQ17, GD11, GSB10, GT13, GGP13, GLPA10, GCZ14, HNI12, HK11, HIC11, HIF11, HHL12, HHL12, HhGq17, IIW11, Iku17, IGMK11, IM15, JPPA10, JN13, J11, JCC12, JSL14, JLZ17, JB11, JW12, JFD10, KM12a, KS11, KWC10, K11, KP11, KB13, KKM13, K11, K12, KK14b, KS17, KZZ13a, KZZ13b, KUTS10, KKT13, KKT14, KG10, KO12, KM13, K11d]. **Study**
[KBMM10, Lan10, LLF12, LGM18, LL13, LKS17, LD14, LP12, LZ10, LCL21, LI11, LW11, LW11, LYP11, LGP11, LNM21, LNP12, LL16, L12, LD17, LW11, L11, LGW11, LC21, LC21, LC21, LC21, L11, LW12, LW12, Lu10, LWC10, LCS11a, LCS11b, LX11, LLC13, LW13, LK12, MY12, MLW14, M14, M17, MAD12, MFS16, MZB13, MFB11, MK10b, MK12, MLC11, M10, MMR10, MCC12, MV18, MP12, M12, MSC10, MO13, MWF11, MUNZ12, MUPC10, M16, M10, M11, MS13, MS17, MHP17, MI1, MK12, M11, MG12, M11, MG12, M11, MTS15, MPCEG12, MMRA10, MML11a, MB12, MBBT12, M13, M13, MG10, MFF13, MSR11, MS13, MCR16, MOH12, ND11, NS10a, NHG12, NDH10, NBL12, NA17, NTN10, NL11, NF11, NHB12, NRCS11, NRS11, NRP11, NRR11]. **Study**
[NJ12, NIT16, NZAV10, NEEV15, QAC17, OPC17, OH12, OH13, OCB10, OPP14, OMD13a, OM13b, OD12, OD16, POL12, PS13a, PEA12, PTS11, PDNC14, PM16, PE11, PW10, PK13b, PKK14, PRG10, PAD10, PRPU13, PM17, Puz10, QHS11, QCW12, Qu13, RYM12, RF12, RGPZ13, RR10, RS12b, RSN12, RMS12, RD14,
RGST12, RYW+15, RCM10, RJLPGH+13, RDM+11, RERE10, RNB+10, 
RS11b, RRB12, SF13, SIT+12, SK14, SD16b, SBEH11, SSK11, SVRLG12, 
SB10a, SKHN13, Sat11b, Sch12a, SK17b, Ser11a, Ser11b, SLS+14, SKS11, 
SHL+13, SLSZ13, SHE10, Shi13, SL10, SMK11, SM13, SR13, SSTD11, 
SLA12, SK11, SSP+17b, SMA11, SZ11, SBB16, SZZ11, SZZ+12, SLZH12, 
SHW+13, SMGZ13, SK10, SYQ+10, SWS12, SWS+14, SZZ+15, 
SYY16, SCZH16, SS13, TK16a, TV13, Tav11]. study 
[Tav12, TM13, TT10, TDOD17, TU10, TLY10, TPS12, TJS17, 
TFA10, TSH17, TFB11, TCC10, TGA+11, Tug13, TWR15, TPT+13, 
UKF+11, UMS13, VF13b, VFPC12, VFC17, Var11, VHTEG15, VVN+16, 
VLN+10, Ven12, VSMK13, VSMK15, VV12, VV13, Vic17, Vik13, VGD13, 
VO11, VO12, WML10, WXZ+11, WJL+11, Wan11, WvRSW+11, WLL11, 
WLG+11, WLWT12, WLZ+12a, WLZ+12b, WWHZ13, WSH+13, WHY+14, 
WVJ15, WTW+15, WD1+17, WWQG17, WZZ10, WTZ+11, WWX+11, 
WLD+10, Wu11, WSL+11, WZC+12, XNL+14, XX12, XSLF12, XLLZ10, 
XZCH11, XZ11, XW11b, XGH+18, YM12, YM13, YYS15, YY18, YZL+11, 
YZZ15, YZ12, YZZ16, YLZ+17, YZ10, ZKRR11, ZSAP11, ZSASS13, 
ZAE10, ZLR15, ZWW10, Zha10, ZLSS10, ZW11, ZLZ+14, Zha14, Zha15, 
ZLWL16, ZCX+16, ZKW17, ZSQ+10, ZRR+11, ZPB12, ZSS+13, ZLWZ16, 
ZTC11, ZQXP17, ZLY+14, ZPB12, ZBB17, ZDZ11, dSS11a, dLRR11, 
BVP13, SW12].

Sturmian [FRGC10, SS12]. styrene [DPDR11, MCC13b].


subsidiary [LWY13]. Subspace [TG16]. subspaces [TLC+17].

Substituent [EHKD11, EEMSS14, MKHM11, Ry12, YR+11, dSNBG08, 
DWW15, EAV16, JNY17, Val17, XX12, ZYL+13, ZBB17].

substituents [AG10a, AMK10, LZZ+17, SN11, WLC+17].

substituted [AAA12, BG13, CLXZ12, EHKD11, EKD12, IGMK11, IUMVB10, JLL11, 
KMM17, NAK+17, ZNAR10, PS13a, PSK+13, SSKS12, SN12, SMGZ13, 
SZL+14, SC18, TT10, Tug13, VSN+11, ZLY+14].

Substitution [SPIL14, Buc10, Buc11a, Buc11b, EMS16, HLJZ11, JLG+12, ND10, RFN+12, 
Rl10, RB11b, dAB17]. Substitutional [BSO11].

Substrates [dSSdS12, FBD+13]. subsystem [MA10, NS10b, Sha11a, YKN13, ZS11].

subsystems [GHP11, HS11c]. subunits [Sch15]. subvalence [dCDC+11].

Successes [Swa13]. successive [SM14b]. such [Ser11a]. sudden [CLXD15].

sufficiently [MK10a]. sugar [BS14, SKM11]. sulfone [CAP12, FMP+17].

sulfate-methane [CAP12]. sulfated [MCRS16]. sulfenate [ZAE10].

sulfdide [BAP13, DWW11, JAB12, MA11a, MTS15, SS14, TCS12, 
YGLL10, YLY+17]. sulfonamide [TPdMB12]. sulfone [FBD+12, ZAE10].

sulfur [CK17, DI11, DSF17, GFRdG11, GCD13, LKd+16, NFD+10, NFQ+11, 
Oni12, SF12, SCB+14, dLDAD12]. sulfur- [NFQ+11].

sulfur-containing [NFD+10]. Sulfuric [dLDAD12]. sulphonamides
[EAK+10a]. sumanene [ONK+13]. Sup [LJ16]. super
[Man16, MBSAG16a, MBSAG16b]. super-resolution
[Man16, MBSAG16a, MBSAG16b]. superacids [CS18, Val17]. superalkali
[TL15, WCY+10]. superalkalis [STM18]. superatom [YLWrL12].
Superatomic [MCK17, MC18]. superatoms [TFB11]. superbases [ÇT14].
super-resolution [Man16, MBSAG16a, MBSAG16b]. superacids [CS18, Val17].
superalkali [TL15, WCY+10]. superalkalis [STM18]. superatom [YLWrL12].
Superatomic [MCK17, MC18]. superatoms [TFB11]. superbases [ÇT14].
super-resolution [Man16, MBSAG16a, MBSAG16b]. superacids [CS18, Val17].
superalkali [TL15, WCY+10]. superalkalis [STM18]. superatom [YLWrL12].
LCCH11, Lru13a, Lru13b, MR11, MFM18, NMIP14, QSX+15, RNdA+10, SW10, Tou13, VLK+11, Xu16, ZK12. Systematic [KSS12, WR15].

Systems [GLT13, IA13, KBF+13, ONK+13, ARG11, Bae16, BR08, BR12a, BBB+12a, Brä11a, BDPT12, BWE16, BBA+16, Cap16, CH17, CS13, CP11, CP16, DAB12, DLRMFY10, DCDD10, Dun15, DB15, Fin16b, FST16, GB10, HS11a, HITU16, HFDGC14, HKLW13, IFT14, JE10, KH12, KKL, KHa16, KCC13, KSD10, KSN+10, KYH+13b, Kon11, Kry11b, Kry12b, Lad14, LS17, LV16, LGZC15, LzD+11, LNI12, MANP17, MC11b, Nag16b, NKF+13, NDH10, NGS11, NYS+10, NMV+14, OPC17, Per10a, PBB15, QTCL10, RB08, RB11a, RABM18, RAGM10, Roy15, RS13, SLG11, SBAT16, SSK11, SMV11, SK17b, SHKS15, Sko16, SKV12, SMPT13, Swa13, TFSRM11, Tok16, TC12, WCM14, XTLA13, XTLA14, YYI+12, YWH12a, YWH12b, YFY17, Zak16, ZWE12, dGR14, dOR10].

T systems [Mam14].

T [BL12, CPF+11, SLS+11, GWM11, WLL+13, BBM17, SD13c, YGLL10, dOR10]. t-cell [WLL+13]. T-junction [SD13c]. T4 [DFF+13].

table [Gar08, GI10, Kut10]. Tables [Rus14].

tartaric [GbZA10].

tailoring [MMA10].

tame [DB13a].

target [HM10b].

targets [PUH+11].

tautomer [LCZL11].

tautomerization [JS17]. Tautomeric [SOM10, CCL+10, JN13, LDW+11, NRS+11, NJA+12, TSH17].

Tautomers [HS11b, PS13a, VF13b].

targeting [MBM10].

targets [PUH+11].

tap [KAOB11, LCH14, Tav11, Tav12, ZR13].

Tayloring [PJP08].

TB [ZCP11].

tBu [HHL12a, HHL14, PP14].

Te [ZLY+14].

TCDD [WWX+11].

TCNE [TD11, KBMM10].

TCNE-methylsubstituted [KBMM10].

TD [AFC+10, BDR12, JPPA10, ACF+11, BVCAP12, FPRGMB12, Kl15, LJ13, Mas10].

TD-DFT [Kl15, LGS+16].

TDDFT [WKE17, BGD14, ESDO16, HKLW13, IHG10, LY11, LZ10, MMWA11, PJP08, PSK+13, VSN+11, YZW+15a, ZAP11].

Tea [MKHM11].

technical [MMP11].

technique [KdSM+10, LKK13, SR12, SOF+10].

techniques [DW12, LSR+10a, LSR+11, MQ13, Ols11b, RW11, SK12].

Technology [YSA+11].

Teller [DMAB12, AGPDZ13, DMAB12, GBF12a, HR12, HFZ12, JZP17, RGZPD13, SBD+16, TPCJ+12, YFY+13, ZFC12].

Teller/Renner [DMAB12].

telluride [KG08, MW15].

tellurium [ESDO16].

temozolomide [KdPNNS16, KMMS17].

Temperature

[Buc12a, KKH+13, MKSG13, PMMGL+11, Boe12, CAA12, CS17, Dun15, KAR12a, MOH+12, Nag17, TD11, WCGD12, ÁFV12].

Temperature-programmed [ÁFV12].

temperatures [Chu12, STM17].

tendencies [SMP10].

tensor [SPM+15, Fin14b, JMX+15, Lya14, NIT16, XXJ+16].

Tensorial [SD13c].

tentative [YFY17].

terephthalate [TIN13].

term [IIH16, Ols11b, ZLJ11].

terminal [SLS+15].

terminated [dLdODAD12].

Terms

[Gin10, Glu13, KL11, PE11].

ternary [MS14b, OGvSG18].

tert [AMAC12].

tertiary [MMM+12, PCML08, SAG13].

test [DA16, Mar12, PWP13].
tetraphenylimidodiphosphinate [SLS]

tetrahedral [IIW+11, MPRB+10, Pup11a, RFGEP+16, TGA+11, WWQG17, YGLL10].
tetrahydrofuran [dSdSPG11].
tetral [DKS11, DKS11].
tetrafluoroborate [MFK+12].
tetrafluoromethane [dOR10, JLL].
tetrasulfonate [DZO12a].
tetrafluorobenzene [dOR10, JLL].
tetraalkane [dOR10, JLL].
tetral [IIW+11, MPRB+10, Pup11a, RFGEP+16, TGA+11, WWQG17, YGLL10].
tetrahydrofuran [dSdSPG11].
tetranitride [DKS11, DKS11].
tetrel [WLC+17].
them [WXB+11].

Theobroma [dAGNTJ12].

Theorem [GW13, Lev10, Nag10].

Theorems [LB14b, Tch16, ZWE12].

Theoretical [YOS15].

Theoretical [Ayp14, AM10, AM12, Ali14, AIGVZW12, ACMRN10, AAA12, AMAC12, BD12, Bar16, BAMA12, BGMD15, BS11, BZZ15, Boe12, BMF13, Bra14, BLM+12, BWE16, CMR13, CWF11, CAX+11, CPL15, Cas15, COCF+14, CNSK11, CWZ+10, CTW12, CWB+13, CWS15, CS18, DIOG12, DSCO+13, Den13, DSRGD12, DSWL11, DWGX12, DSH+13, EAK+10a, ESDEO16, FM16, Gao12, GZW16, GK12, GDDNGS12, GIO12, GFB12b, GMT16, GDM+10, GSB10, HTM10, HK11, HEC+11, HDQ+13, HLMO11, HMM+13, HLJZ11, HZG12, HHL12a, HWL16, HM10a, HWHZ11, IIW+11, IGMK11, IROW10, JFT13, JSLH14, JLZ+17, JWQ+12, JFDD10, KSI1, KB13, KWC11, KA13, KI12, KSSK16, KSY+11, KZZ13a, KHH10, KAOB11, LKDC11, LHO13, LJ16, LCL+10b, LZB10, LPO+11, LMZ+11, LPG+12, LSR+13, LXW+14, LGZC15, LD17, LL+11, LWJL10, LDW+11, LXW+12, LWZ+14, LZZ+17, LWJ+12, LW+12, Lu10, LW+10, LMCZ11, LCLZ11, LCS+11a].

Theoretical [LCH+11, LCS+11b, LXX11, LW13, LD+18, MLW10, MWH15, Mas10, MOY13, MNDNO+16, Men10, MAP+10, MSK11, MJ14, MMHP17, MGD11, MBBT+12, Mor11, NYA+13, NL11, NM14, NFD+10, NFQ+11, NH11, NBH12, NTF16, OT14, ONK+13, PEA+12, Pan16, PPK14, PMC11, RNF+12, RMLPGGH16, RCM10, Riv11, RGS+13, SK12a, SRAZ16, SLS+14, SLZ13, SZZ11, SLZH12, SM14d, SK12b, SK10, SLS+15, SZL+15, SCZH16, TYN13, TWHZH14, TM13, TYL10, TXL10, TSH17, TFB11, TGA+11, TPT+13, UFK+11, VF13b, WXZ+11, WLL11, WLG+11, WTH+11, WLZ+12b, WHS+13, WHY+14, WTW+15, WWQG17, WHM14, WZZ10, WJ11, WSL+11, XZL+12, XWC11b, XXbX+13, XCY15, YZ13, YZL+10, YJ17, YHLC15, YCL13, Zha10, ZZX10, ZLLS10, ZYZ+11, ZZR+12, ZSHL14, Zha14, ZQW+11, ZYSW17, ZSQ+10, ZFS+11, ZL12, ZSS+13, ZTC11, dSdSPG11, dARAV12, dOdONM12, AZD+11, ASD14, BLL+13, BLRD+10, BG13].
theoretical

[BP5M12, Buc10, CZJZ12, Caol7, CG12, CYLL11, Che12, CLH14, CGIAI12, CPAT11, DDCY12, DPRK12, DTEMK11, DZI1a, DQZF12, DC12, EI11, EMED12, ENV15, FMP17, Fri12, GLF12, GHGF12, GT13, GGP13, HYZ13, Iku17, Jal10, Jia15, Kim16, KO14, LS17, Lan10, LRP11, LL11, LCZ15, LLZZ10, LXD13, LW15, LdAA11, MCP10, MMR10, MPTR12, MLPT10, MUPC10, MEF15, MEO13, MSO13, ND11, NGH12, NBL12, N`em14, NRS11, OH12, OH13, OKR12, ORJ18, POL12, PM17, Puz10, RGR12, SFL10, SSK11, SIS10, SKY13, TKN13, TH13, YSS10, YKN13, YH14b, AM13b, AGPDZ13, BVP13, BGBV12, BLKB11, BjdIMAV12, Cam12, CCL13, CEFMK12, Cha11, CH17, CM12, CZLD17, CK17, CFI14, CTDOL01, CST16, DWJZ11, DCBB11, DKS11, DLRMFY10, DB11, DMVW11, DGR16, DCH11, FZX18, Fin17, FA17, FMMD10, Fri12, FSST16, GCK17, GM11, GEL18, GS11, GCZ14, HLZ14, HMM10a, HMM10b, HKIH13, HYD11, IN15, IROW10, JR12, JPP11, JMX15, JW18, KAR12a, KCD15, Kar13, KKL16, KS11, Kit14, KM12c, KdSM10, KJ14, KMU13, Lar12, Lat13, LPO12, LCL10b, LW11, LWL12, LPG12, LBY14, LLW11, Lin14, LDZ16, LLZ12, Lya14, LKd16, MZX10, MLY14, MJ16a, Mam14, MLC12, Mas14].

Theoretical [DJB10, DC10, HHL14, LEU11, Sit15].

theoretical/computational [N`em14].

theoretically [Jeo18, VMC11].

theories [Cam10, JNZ14, Luz08, ZT13]. Theory [Anol3-49, Buc12b, DCZ17, HKLW13, ISN13, IKN13, Koc13b, Kut13, LMZ15, MIN13, NS13, SSI10, SSS10, SKY13, TKN13, TH13, YSS10, YKN13, YH14b, AM13b, AGPDZ13, BVP13, BGBV12, BLKB11, BjdIMAV12, Cam12, CCL13, CEFMK12, Cha11, CH17, CM12, CZLD17, CK17, CF14, CTDOL01, CST16, DWJZ11, DCBB11, DKS11, DLRMFY10, DB11, DMVW11, DGR16, DCH11, FZX18, Fin17, FA17, FMMD10, Fri12, FSST16, GCK17, GM11, GEL18, GS11, GCZ14, HLZ14, HMM10a, HMM10b, HKIH13, HYD11, IN15, IROW10, JR12, JPP11, JMX15, JW18, KAR12a, KCD15, Kar13, KKL16, KS11, Kit14, KM12c, KdSM10, KJ14, KMU13, Lar12, Lat13, LPO12, LCL10b, LW11, LWL12, LPG12, LBY14, LLW11, Lin14, LDZ16, LLZ12, Lya14, LKd16, MZX10, MLY14, MJ16a, Mam14, MLC12, Mas14]. theory [MW16, MLK17, MLB01, MBBT12, Mor13, MCRS16, Mur12, Nag15, Nag17, NSN17, NNSN17, Na13, NS10b, NAK17, NTNL01, NL11, NMP14, OK16, OD16, PS01b, PS14, PK13a, PABSK16, PP16, Pat15, PTH11, PR10b, PBB15, PU14, PM16, PJP10, PMAP12, PI16, PC13, RGPZD13, RAMB18, RS09, RS11a, Rud12, SVRG12, SN15, SN12, SZS10, SLZ11c, SLS11, SLM13, SM12, Sto18, SK12b, SD13c, SS13, TFBG14, TIN13, Tan13, TTD13, TH12, TDO17, TG16, TLE17, VPGC12, Var11, VUC13, VBO15, WKE17, WJL11, WW11, WJY15, WB17, WD17, WZ17, XNL14, XGH18, YKM15, YWH12a, YWH12b, ZS11, ZQJC10, ZLWY13, ZCX16, ZM13, ZSZ14, dCSDdMC13, dSHT17, BM10]. theory-based [KS11, WJ15]. there [GI11f, SM14, TKSK17].


Thermodynamic [JAB12, XNL14, COCF14, DWGX12, Kim13, LZZ13,
OSJ⁺12, RMLPGGH16, Tav11, TSH17, dOLdIV13]. Thermodynamical [Nag17]. Thermodynamics [MLW16, PK16, BvWG14, DP11, PD11, PRFR17, WSCL11].

thermoelectric [KG17].

thermostat [GP13a, HCL13, OGvSG18, TFSRM11, XMZ⁺12, ZK12, ZLHY13, ZDZL11].

thiazole [DDC¸Y12, SC12a, SC12b].

thiazol [MBBT¹2].

thiazolidine [VMC11], thiazol [DDCY12, SC12a, SC12b].

thiazolylic [MBBT¹2].

thiatri [LCS⁺11b].

thin [Ril10].

THF [HHL12a, HHL14, AG10b, RTT10].

thiadiazole [VMC11], thiadiazole [VMC11].

thiacyanate [LGS⁺16].

Thiocyante-free [LGS⁺16].

Thioflavin [BBM17].

thiol [JS17, KV11, OD16].

thiol-functionalized [OD16].

thiolate [MC18, OPF11, ZZC15].

thiolate-protected [MC18].

thiols [KV11].

thione [JS17, KKG12].

thiophene [CZLD17, MSG16].

thiophenols [dSNBG08].

thiosemicarbazone [LWH⁺12].

thiourea [LCM⁺11].

third-order [MMF⁺13, NKF⁺13, RS09, RS11a, WLZ⁺12a].

third-row [KWC11].

thoughts [KN15, Lev16].

three-body [ARG11, Hog13, RAGM10].

three-center [Buc10, Buc11a].

three-dimensional [DMS⁺10, MPD⁺15, SD13b].

three-electron [Buc11a, CG12, LWY13].

three-membered [Zha14].

three-peak [HYH⁺10].

three-photon [WLZ⁺12b].

three-state [GSaY11].

three-unit [LQZZ12].

threeonine [WJY15].

three-state [HMH⁺13].

through-bridge [KyH13a, Na12, Na13].

through-space [CDT12, Na12, Na13].

throughput [CRFR11, KG17].

thymidine [MB14].

thymine [TWHZ14, HYD11, TSH17, XSSF12, YM13].

Ti [FTB11, HLMO11, JL12a, MLY⁺16, TFB11, ZLY⁺14, CAZ⁺11, OPP⁺14].

Tietz [KBG17, AAHN16, HRT12].

tight [LNI12, WDJ⁺17].

tight-binding [LNI12, WDJ⁺17].

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Zerbetto:2016:TRM


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Zhao:2011:DFS


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Zhao:2010:TSS


Zhao:2013:TSM


Zazza:2010:CHP


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**Zhao:2015:MCC**


**Zicovich-Wilson:2012:BWT**


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