Title word cross-reference

(001) [dLdOAdAD12]. (100) [MFK+12]. (1 ≤ n ≤ 6) [UDVD10]. (2 ≤ n ≤ 8) [BLRdA+10]. (3 + 2) [WLS+19]. (3 + 3) [LFTL18]. (A = N, B) [ASW13].
(k + l + m = 4) [KYLC19]. (m + n = 3) [UKF+11]. (m = 5, n = 2) [MHHPR+17]. (m = 6, n = 3) [MHHPR+17]. (n = 1, 2) [Men10]. (n = 1, 2, 3) [EML+11]. (n = 1 -- 4) [LL11]. (n = 1 -- 7) [CAZ+11]. (n = 2, 3) [DTEMK11]. (n = 2 -- 10) [WJL+11]. (n = 2 -- 34) [QSLY10]. (N = 28) [GD11]. (r, s) [Bib13]. (ϕ - ψ) [MAW+18]. + [Buc12a, CdAFS+12, DMAB12, FRNM12, GKT+12, KT12b, LWZ13, MEEA+13, MPRCEG12, MOH+12, RSN12, SABA+12, SD12, WZH13, XZL+12, YGL+11, YZ10, ZH12]. 1 [BEM12, DFK16, JW19, PSKV19]. 1/3 [KLZQ15]. 13 [LXD13]. 14 [YD17]. 16 [GAPK+19a]. 18 [YD17, GAPK+19b]. 13 [GWZ+14]. 2 [ABTW14, CPL15, HMA+19, HGB08, IK14, LLZaH14, LD17, NF11, PSKV19, SPD+18, SdS17, YSW11]. 2(N + 1)^2 [MC18a]. 2n [BBYZ18].
\[2n + 2\pi \] \[MB13\]. \[2n = 68, 70, 78, \] \[WLZ^{+12a}\]. \[2p\pi \] \[VLFG12\]. \[3] \[ABTW14, BMX^{+19}, GWJ12, KSO^{+19}, LQZZL12, LD17, RLW^{+13}, SM^{+14c}, VVY18\]. 30 \[GGD12, SLZ^{+12}\]. 3d \[ALA15, DD17, RZC13\]. \[3\sigma \] \[VLFG12\]. \[4] \[ABTW14, CD12, GAPK^{+19b}, GB13, GWJ12, HCL13, LKN13, SM^{+14c}, WLS^{+19}\]. \[4\sigma \] \[VLFG12\]. \[4f\pi \] \[VLFG12\]. \[4f\sigma \] \[VLFG12\]. \[5] \[ABTW14, BGMD15, BJD1MA12, CSDK12, HDQ^{+13}, MPE15, SM14d, SM16\]. \[5g\sigma \] \[VLFG12\]. \[\leq 5 \] \[LCZ15\]. \[6] \[CWSZ13, HDQ^{+13}, LdMcDA^{+12}, MPE15, MJ14, MMV^{+19}, PAI18, PAKA15, SS18a, VBO^{+15}\]. \[6; y = 1, 2 \] \[BCGC12\]. \[6i\sigma \] \[VLFG12\]. \[6j \] \[RBO^{+10}\]. 7 \[CHV14, GGJD13, SR13, WCS^{+13}\]. \[7\pi \] \[KMF^{+11}\]. \[7\sigma \] \[KMF^{+11}\]. \[8] \[YC13\]. \[8\sigma \] \[KMF^{+11}\]. \[8\sigma \] \[KMF^{+11}\]. \[8 \leq n \leq 14 \] \[NW12\]. 9 \[AIi14, SB16\]. \(< \) \[BTH18\] = \[BPG^{+10}, BL10, BDK12, CF\text{C}11, DIOG12, DPPR11, ESS13, FTB11, GB13, JLI12a, KyH13a, LZZ^{+11}, LMZ^{+11}, LLG^{+12}, MLW10, MPPR^{+10}, dMOB12, QU13, SZZZ11, SYQ^{+10}, SZL^{+14}, TFB11, WCY^{+10}, WSL^{+11}, XZZ^{+10}, XWC11a, XWC11, YK11, YIY^{+13}, YL11, ZQJW13\]. \(> \) \[BTH18\]. \[2 + 2 \] \[MBS^{+18}\]. \[2 + 4 \] \[LLF17\]. \[2, 7 \] \[WWL^{+11}\]. \[2n, 2 \] \[LS13\]. \[3 + 2 \] \[ZRG^{+19}\]. \[3 + 3 \] \[ZQW^{+17}\]. \[4 + 2 \] \[HHZ^{+19}\]. \[4 + 3 \] \[XZG^{+18}\]. \[< \) \[ADB10, AGRI^{+12}, BD12, BCK19, BHV^{+11}, Ber13a, BGI11c, DW1Z11, DZ11a, DCHL11, FB11, WWL^{+11}, HCL13, LKN13, SM14c, VVY18\]. \[= \) \[BPG^{+10}, BL10, BDR12, CF\text{C}11, DIOG12, DPPR11, ESS13, FTB11, GB13, JLI12a, KyH13a, LZZ^{+11}, LMZ^{+11}, LLG^{+12}, MLW10, MPRB^{+10}, dMOB12, QU13, SZZZ11, SYQ^{+10}, SZL^{+14}, TFB11, WCY^{+10}, WSL^{+11}, XZZ^{+10}, XWC11a, XWC11, YK11, YIY^{+13}, YL11, ZQJW13\]. \(> \) \[BTH18\]. \[2 + 2 \] \[MBS^{+18}\]. \[2 + 4 \] \[LLF17\]. \[2, 7 \] \[WWL^{+11}\]. \[2n, 2 \] \[LS13\]. \[3 + 2 \] \[ZRG^{+19}\]. \[3 + 3 \] \[ZQW^{+17}\]. \[4 + 2 \] \[HHZ^{+19}\]. \[4 + 3 \] \[XZG^{+18}\]. \[\neq \) \[ADB10, AGRI^{+12}, BD12, BCK19, BHV^{+11}, Ber13a, BGI11c, DW1Z11, DZ11a, DCHL11, FB11, WWL^{+11}, HCL13, LKN13, SM14c, VVY18\]. \[\neq \) \[BPG^{+10}, BL10, BDR12, CF\text{C}11, DIOG12, DPPR11, ESS13, FTB11, GB13, JLI12a, KyH13a, LZZ^{+11}, LMZ^{+11}, LLG^{+12}, MLW10, MPRB^{+10}, dMOB12, QU13, SZZZ11, SYQ^{+10}, SZL^{+14}, TFB11, WCY^{+10}, WSL^{+11}, XZZ^{+10}, XWC11a, XWC11, YK11, YIY^{+13}, YL11, ZQJW13\]. \[\neq \) \[BTH18\]. \[2 + 2 \] \[MBS^{+18}\]. \[2 + 4 \] \[LLF17\]. \[2, 7 \] \[WWL^{+11}\]. \[2n, 2 \] \[LS13\].
LKN13, MHPR+17, PAPCMM+16, UKF+11]. N
[DVDBM11, EHK11, EK11, GGD12, GD11, LJK+18, MEEA+13,
RWW+19, SM16, Ali14, BPG+10, BGM15, BEM11, BLRdA+10,
BJdIMAV12, CDSK12, CAZ+11, CTW12, CWS13, CD12, DTEMK11,
EML+11, FTB11, GR11, GAPK+19b, GGJD13, GP13b, GB13, GWJ12,
HDQ+13, KSSK16, Kuz19, LRKM10, LKN13, LGHL11, LWL19, LCZ15,
LHL+15, MCP10, Men10, MJ14, MMV+19, MHPR+17, MMRRA10, NW12,
PAKA15, PAPCMM+16, QSLY10, RGR12, SKS10, SJZ+18, SR13, SBB16,
SLZ+12, SM14b, SM14c, SM14d, UKF+11, UVD10, WJL+11, WCS+13,
WJL+10, XYL+18, YC13, ZRR+11, ZCTG18, ZCP11]. n-1 [MCP10]. n-2
[LCZ15]. [(n-4)-] KMM16. N [RWW+19]. n-0/2-
[DHYC19]. 2+ [LL18]. 2- [SM14c]. x
[BCGC12, GLF+12, HCL13, KA13, On112, RLW+13]. y [BCGC12]. A
[ASW13]. α [BWBP+18, HZZ+19, KSAK17, MFZ+18, OPAVM18, LZZ12,
PEA+12, QTCL10, SVRGV12]. α2 [EPS+16]. β
[AC19, GZZ+14, JEC018, JSLH14, KZZ13b, LSG+14, OPAVM18, WSH+13,
NHFPVG12, NRP+11, PEA+12, SJW13, TPDMB12]. β2 [CSVCB12].
[BLW17, BTH18, XF19, Men10, TBH11, XLGA12]. … [TG13, JLG+12].
[IIH16, PGGMGM15, CWW+16, MVG18, MW16, OVT+16]. d10 [DLJT14].
Δ [CC11b, Yam10]. Δex [DE18]. [ZHF12]. [VLM+10]. [MSBF18]. η5
[DZO12b]. f [MW16]. G [ATPR11, DKS11, VATPR11, VAT12, SPO+11]. γ
[BWBP+18, CC11b, MFK+12, PEA+12]. h [PUGSF18]. J [AAHN16]. j = 0
[LZF13]. k(T) [CP11]. K+ [GBK18]. K2+ [GBK18]. l [WC14]. l + m + n = 6
[PAPCMM+16]. 0 [PAPCMM+16]. λ [AM13a]. λ5 [TM19].
LDA + U [HFDGC14]. ← [SB18]. M [XYL+18, KC11]. m, n = 1 [LKN13].
m = 1 [CD12, GWJ12]. m = -2 [FTB11]. m* [Dw13]. M5V [HNBS18]. μ
[ESS13]. N
[CZJ12, CPL15, DDÖY12, DPRK12, DDF+12, ES17, GW18, KC11,
KSAK17, MOSK10, MAN15, NJA+12, Pan16, RWW+19, SFW12, CMCN11,
CS12, DFK16, DHYC19, GE12b, KSSK16, KMM16, LWL19, ZYZ+11].
n + m ≤ 5 [CD12]. N, N [DAVMD17]. n = [LHL+15, SM14b]. n = 0
[GAPK+19b]. n = 0, 1, 2 [SKS10]. N = 1
[SM16, CWS13, GGJD13, GB13, HDQ+13, SR13, SM14d, WCS+13, YC13,
BGM15, PAKA15, SBB16, SM14c, BJdIMAV12, CD12, GWJ12]. n = 1, 2
[BPG+10]. n = 1, 4, -7 [FTB11]. n = 2
[Ali14, HDQ+13, MJ14, MMV+19, CDSK12, GGD12]. n = 2, 3, 4 [GP13b].
n = 20 [SLZ+12]. N+ [CZJ12, DDÖY12, TYD11]. n ≥ 2 [SM14c]. o
[KSAK17, SR18]. p [AGJ12, AMAC12, CS12, DLJT14, HLZ+14, RRK16,
SR18, SRA+11, ZSS11, ZYZ+11]. π
[BWE16, CCS13, DWZZ15, HIL19, KPL+17, LDKB15, LW18, LB18, MC17,
MAN17, NCMM+18, NIK19, NMV+14, OCGM+19, PC16, PNC19, SSB19,
SPD+18, SSS15, Szc18, TK16B, YZZ16, YD17, ZHL+19, CC11b, SLS+12,
AEKGZ12, BMR+13, DB15, FV11, GNMI+12, LCB10, MMA10, Nik11, NRGS11, RVNP12, RNVi+12, SD13a, VS11, Yam10, ZZZ+11. \( \Pi_a \) [HIL+12b]. \( \pi \cdots \sigma \) [WLC+17]. \( \pi \sigma^+ \) [KGV11]. \( pK_a \) [PWH+18]. \( \tau \) [Dau16, SAHAA16]. \( \Phi^\circ \) [GSI10]. \( q \) [Agb12]. \( q = 0 \) [SM14c]. \( \rightarrow \) [Buc12a, Coo12, GKT+12, LCB10, MPRCG12, NWQX11, YGL+11, YZ10, ZH12]. \( \rho \text{SU}(2) \) [Bra10]. S [HR12, MMM19]. S = 1/2 [KZQ15]. \( \sigma \) [LW18, SPI14, SC18, ZHL+19, CC11b, Ang10, Che12, DCDG10, JLG+12, Yam10]. \( \Sigma^- \) [SL5+12]. \( \sigma_{\text{hole}} \) [VJ15]. \( \sigma \pi \) [ZXY13, DMWH11]. \( sp^2 \) [OCGM+19, PNC19]. \( \sqrt{3} \times \sqrt{3} \) [OD16]. \( T \) [XCL+18]. \( \times \) [PWL+10, ZHY10]. \( \rightarrow \) [GW18, KMM16, ZWL18]. \( v = 0, 1 \) [LZF13]. \( v = 0, j = 0 \) [YZ10]. \( \varphi \) [CC11b]. W(\( l, m, n; \alpha, \beta, \gamma \)) [LWY13]. \( \wedge \) [ZQJ13, LYD+12]. X [AGOP18, AM18, BHA19, Kuz19, SB18]. x = 0 [HL13a]. x = 1 [RLW+13]. x = 2 [BCGC12]. X- [Kuz19]. X2 [BHA19]. Y [Kuz19]. Z [XCL+18]. * [LCB10].


2 [Boe12, EKD12, KK14a, LJK+18, LV12, Men10, MEEA+13, SAHA16, Tan12, WWX+11, Zha14].
2-adamantyl-thiazolidine-4-one [MBBT+12]. 2-amino [RJY+10].
2-amino-3-methylimidazo [MLPT10]. 2-azidoethanamines [SM10b].
2-dichloromethylbenzimidazole [PMC11]. 2-dihydro-3H-pyrazol-3-one [TAY11]. 2-dione [OPP+14]. 2-dioxetanone [dSdS13b].
2-ethoxypyridine [MCC12]. 2-furoic [GIO12]. 2-hydroxy-3-methylbenzylidene [TAY11].
2-pyridone [HHCA10, MCC12]. 2-RDM [KK14a]. 2-substituted [Tug13]. 2.0
[CW+16, LKZ+16, SC12b]. 3- [SC12b]. 3-alkylthiophene [BMR+13].
3-aminoacrylaldehyde [NRS+11]. 3-bisphospho-D-glyceric [SLA12].
3-dihydrolutidine [TM13]. 3-dimethyl-aminobenzonitrile [NMHPVG12]. 3-dimethylaminophenyl [FO10].
3-mesityl-3-methylcyclobutyl [KDC+12]. 3-methyl-1-pyridin-2-yl-5-pyrazolone [PGG12].
3-methyl-3-phenyl-cyclobutyl [SC12a, SC12b, DDČY12]. 3-methyl-4-nitropyridine [KC11]. 3-pentafluorophenyl [SM10b].
3-phosphonothioic acid [LYH+11]. 3-phosphonothioic acid-2-carboxylic acid [LYH+11]. 3-phosphonothioic acid-3-carboxylic acid [LYH+11].
4-trifluoromethylphenyl [SAHAA16]. 4-X-2-hydroxybenzaldehydes [EKN10]. 400K [KAR12a]. 4965 [SKHN13].

5


9- [CRSB12].

= [AGOP18, AM18, BLL+13, BHA19, BBYZ18, CWS15, CDL+19, DPDR11, DD17, DHYC19, EMSB15, EMS16, EAV16, GWML11, HNBG15, HNS18, HWL16, JLG+12, KSSK16, KMM16, Kuz19, LJI+11, LC16, LL18, LWL19, LG11, LXD13, ML1+16, MLW10, MZLM17, NBL12, PSK+16, PP19a, Pan16, PCD14, PAKA15, RWW+19, RBTL19, SB18, SMC18, SSK10, SPL14, SM17, SYQ+10, TW10, TL15, VO12, WSML16, WZW17, WLL19, XYL+18, XZL+12, XCL+18, YLWL12, ZHL+19, ZCTG18, ZLY+14, dOR10]. =4 [BEM11]. =H [RLTAT19].

activity
[BD14, Hat13, MPMCM+11, RCM+19].

acute
[ASD18, BGJSM+18, CJZJ12, CWL+13, CjongTL12, DSD18, DMBJ15, ESBJYJ12, GTSC+19, HSYM11, JB11, LCG12, LWH+12, MLC+11, PGG12, RCM+19, SHTO11, SS+12b, ZYL+13].

acyclic
[BBKO16].

acylbenzothiazolon
[SSTO11].

acylhydrazones
[Cao17].

acylium
[FDMR11].

acylphloroglucinols
[KM12b, MK10a, MK12].

adamantane
[BBKO16, GZ14].

adamantane-based
[GZ14].

adapted
[Ali19b, ANC+15, CB10, SR12, TPCJ+12, VRO+12, WH12, YKN13].

Adaptive
[BG11a, BR15, Lya14, MBSMJC18, ZKW17].

adatoms
[PP10, WDJ+17].

added
[Fuk12].

addition
[DI11, Buc11b, CAAI12, DP12, DFK16, Dum12, GW13, GMT18, JSLH14, LCM+11, LW13, MNC18, PDC14, SHL+13, SDR+13, TIN13, TBHL11, WZL+10].

addition-substitution
[Buc11b].

additions
[SFW12].

additive
[KF19].

additives
[YZZH15].

Addition
[BMB16, RLER10, Dob14].

address
[VVJ15].

adduct
[DWGX12].

Adducts
[BAB+18].

adenine
[MYZ+10, SOM10, TSH17, XSLF12, YTY19].

adenine-thymine
[XSLF12].

adenine-uracil
[MYZ+10].

adenosine
[DSWL11, PRG+10, WYWL13, YTY19].

adenosylmethionine
[WYWL13].

adenosine triphosphate
[KTI+12].

adrenoceptor
[CSVCB12].

adsorbates
[BWW+10, LRKM10].

adsorbed
[Hog13, JCCZ12, RFMC19, TTM16].

Adsorption
[CA17, DI18, IK18, NA12, SQ10, UDS19a, UMS13, BGMD15, BAP13, CTW12, CA018, EO11, EO11, FFF10, FTB11, GP13b, HZL+14, HCL13, Kim18, KF17, LV19, LZ12, LWX+14, LIK15, NBL+14, ONBP11, PK16, RD14, RJLPGH+13, SD16a, SR19, SM19, VSMK13, VDG13, WJY15, WLM+19, WZC+12, WH18, ZDL11, dLdOAd12, GD11].

adsorptions
[FZH+18].

adsorptive
[HCH+18].

Advances
[AK11, MCCGM+19, Nag16a, Liu15a, Ped16, Ban12, Mor13].

aerobic
[KBF+13].

aerogen
[KBF+13].

aerogen-bonding
[EAV16].

affected
[VGS10].

afects
[GJ18].

affinities
[DTMK11, KKT13, KKT14, VF13a].

affinity
[CSSK+12, DPK18, DJ18, ESLM19, KKM+12, Kry11b, Kry12b, Shi13, dCSdMC13].

after
[GD11].

Ag
[MSOV13, OD16, PAPCMM+16, SZZZ11, SYQ+10, XWC11a, ZPR10, AGG+18, ESBJYJ12, JFT13, LRKM10, PSK+16, RK14, SQ10, WLL19, ZRR+11].

against
[FMP+17, GAI19, KF19, SBKJ18].

AgBr
[RS12a, RS12b].

agenda
[SG14].

agent
[MBI4, PPK+13].

ages
[Nic14].

aggregates
[ATS+11, TFB11, WKE17, ZLE17].

Aggregation
[YLM+19, GDM+10, MAD12].

aggregations
[BBKO16].

AgOH
[KSST12].

agonists
[Ser11a, Ser11b].

agostic
[HHL12a, HHL14, WLS+19].

AgSi
[ZCP11].

ahead
[HJK14].

AHHC
[dOR10].

aim
[GWZ+14b, NRHJ11, PK13a, RJJY+10, RJA+10, UDVD10, ZZL+11].
Aiming [BBB16]. Al
[CWS15, CDL+19, HHL12a, HHL14, JLL11, LX1313, MLW10, MFK+12, Oni12,
Sat11b, TW10, XWC11a, CRB+12, DCDD10, DSZB18, KYLC19, LLZZ10,
MCP10, NH11, Pan19, Sat11a, SUL+11, TZD+19, VDG13, WJL+10, PS13b].
Alanine [VO12, ZPR10]. AIB [RRRV19]. alcohol [Pli18, SCL19, dCDC+11].
alcoholamines [LCT14]. alcohols [MMM+12, SGK12, SK12a, ZZC12].
AlCoN [AAAM12]. aldehyde [AG10a, LCS+11a, PWH+12, ZSS+13]. Alder
[CM12, Iku17, LW11, MIKH19, ZLWL16, ZXY13]. aldose [SSdS17].
adose-ketone [SSdS17]. Algebra [RW12, Lya14]. algebraic
[SCLCPB12, SÁBA+12]. algebras [WH12]. algorithm
[AFM+10, CGG18, GI11d, IG11, MCP10, SGH10]. algorithms
[CL08, TB15]. AIH [NH11, SLZ+11c]. aligned [HV11]. alignment
[CLL+11]. aliphatic [PI13, SN11]. Alkali
[CFC11, Ber13a, HWL16, HWWW18, SHE10, SM14c, UDS19a, UDS19b].
aklali-atoms [UDS19a]. alkali-based [UDS19b]. alkalide [SM17]. alkalides
alkanes [GZBH18]. alkene [ZSS+13, ZFW+13]. Alkene-3-quinolincarbonitriles
[ZFW+13]. alkenes
[CAA112, KB17, YZZ16, ZYSW17]. alkyl [ESS13, LYW11].
aklyaromatics [BMR+13]. alkylation [UMVB10]. alkylidene
[VGGPD19]. alkylithiophene [BMR+13]. alkylnes [LW15, SLS+15]. all-
[HWW18, LCB10]. all-electron [MPD+10, MPZW10, NDM+12].
al-meta! [MLW10]. all-nonmetal [JHL+18]. alkenoates [XZG+18].
allosteric [SKB18]. allophan [KB13]. alloy [BXR+13, VDG13, XGH+18b].
AIN [AAA12, RJLPGH+13]. AlNiN [AAAM12]. AIO [SZ11]. along
[IKS08, IKS10, KRG+13]. AIOOH [MMC+19]. alpha [MBTV12, SLS+10].
Al — [TZD+19]. alternant [DB13b]. Alternative
[CSTA16, COCF+14, GZF14, MJ16a, PCK19, SKLC19, Sze18]. alumino
[Ped16]. alumino-silicate [Ped16]. alumino-silicate [PM10].
aluminosilicates [CDFD10]. Aluminum [ALK18, AGB19, ALK19, HT10,
IIW+11, Kar12b, MMC+19, MS14b, MM11, PMH+16, SM19].
aluminum-bismuth-nitrogen [MS14b]. Aluminum-poor [ALK18].
Alzheimer [Bal16, MPTR12]. Am [PKK14]. AM05 [MA10]. AM1 [PI13].
ambient [Ma14, WC12D]. ambiguity [Fin14b]. ambiphilic [MAN5].
America [CBMMAPR19, MCCGM+19, MCMV19]. American
[GRGRRHT19]. amide [TPT+13]. amido [JLS13]. amido-amine [JLS13].
[HS11b]. amines [KSAK17, LSR+10a, LSR+11, LW15, RZG12, TV13].
Amino [DSCO+13, AM13b, Coo12, CF17, Cza18, DJB10, Jai10, KyH13a,
KSS12, MLPT10, Mit11b, NHG+12, Pog12, QZH13, RJY+10, Ril10, TAY11,
VHTEG15, WHM14, YSW11, ZCC11]. amino-2H-imidazole [VHTEG15].
aminoaconitrile [CdlDSC18, NC11]. aminoacrylaldehyde [NRS+11].
aminobenzenitrile [NMHPVG12]. aminocarbonothioyl [KDČ12].
[AY15, BC15, BC16, BR12b, DVP18, Fin15, GZSMFN16, HMH10a, HVR18, IIH16, Kut13, PCV19, RAN18, SABA+12, SK17a, Sut12, VVN+16].

approximations
[CLXD15, FMMD+10, GZSMFN16, Per18, PBB15, RBD+10, SGL+16].

APSG [JNZ+14]. APSG-based [JNZ+14]. aq [DSZB18]. aqua [BSPK11, MGK19]. aqueous [AMMK11, CTVA12, DZO12c, GCDNGS12, JCC10, KS11, KSS12, LGZC15, MB14, MNE+13, MPL+11, PS10a, RZG12, RCM10, SM10b, TIKN11]. AR20 [CWB+13]. Arbitrary [IAA15, WC14, ZHF12]. Archea [SLS+10]. Archea [SLX13, HMH10a, HVR18, Kut13, PCV19, RN18, SABA+12, SK17a, Sut12, VVN+16].


MFLK11, MAPS18, MNS11, MR18b, Pea11, PSC15, Pup11a, PJ19, RZ17, RZSZ18, RAFFR15a, RAFFR15b, Roy15, Roy16, RRCO11, RR19, SRPD16, SK17a, SKMN11, SL13, SS12, TBB+19, TW10, WWHZ13, Zak13, ZS12.

atom-bond [AD17]. atom-centered [KFS13, Zak13]. atom-pairwise [KKL+16, PSC15]. Atomic

[AST19, Obs11b, PNC19, SV11, ABS11, ALRA10, ALRAE11, CRA+11, CF11, CB10, Fin14a, Fin15, Fuk12, Gra08, Gra11, GE12b, HST13, IFT14, Lai11, LRMAA19, MK+12, Mann14, MC11b, May14, MS17, NDH10, Nic11, NE11, PUH+11, RLER13a, RAGM10, Rom10, SLG11, SMV11, Sch15, SD13c, STM17, TMC+13, ZY13, ZLWY13, ZZZ+18, vLRRK15]. atomic-wire [SD13c].

Atomistic

[AGG+18, Mai14, BMR+13, CLKD15, MMP+18a, vL13, Zha17].

atomization [Vyb08].

Atoms

[LSC+18, OA13, TBRIS12, AMK10, AM10, BHMN19, BAX+19, BSO11, Dil13, DSSM18, EMSB15, GBS17, GLT13, GZSMFN16, GI10, GI11b, GI11c, GI11e, GS11, Gra11, HMP+11, HMA+18, IG11, JEA13, JMX+15, Joh17, Leh19c, LKJ13, LZW+15, LHX+19, LLH15, Luz11b, MOY13, MFLK10, MJ11, NS10b, NT16, ONBP11, OD12, PRPU+13, PWP13, PNC19, RLW+13, RD14, RBVAG18, SBMM11, SBM16, SR19, Sha18, Sto18, SKL10, TBRIS10, TBRIS11, TH12, TXK+19, TFMC19, TLC+17, UGWL18, UDS19a, WLS+19, YJ17, ZS11, ZCG+16, ZHI17, ZZZ+18, ZJS13, dSTH17, dCGAMV12, Leh19a].

Atoms-in-molecules [OA13].

ATP [BGJSM+18]. attached [HMP+11].

attachment [DSVP15, Kry12b]. attack [LZFZ13]. attending [GWME18].

attenuated [NDP10]. attenuating [CF14]. Attosecond


aureusidin [KK11d]. aurones [XLZ+19]. AuSi [BCK19].


autoionization [DE18]. autoionizing [Cor16]. automated [KMNSP19, MHO+15, NKWT19, PBB15]. Automatic [MML+16, CW11].

AuX [LC16]. auxiliary [CEFMIK12, GS10, KFJ+18].

auxiliary-density-matrix [KFJ+18]. averaged [ABL11, CP13, RS12b, RSN12]. avian [KRH13, PCML08, WZ10a, ZBK15].


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

MSNP18, MG12, NDM+12, PCD14, PBR18, RZSZ18, RLER14, RVO+14, RLZ12, SKT15, SXH18, SZS+10, SLZ+11c, SLZ+11a, SLS+11, TCG17, TWR15, UGW18, UV18b, VSS11, VRO+12, WSV10, YMI14, Zak13, ZF15. 

SBD\(^{+16}\), SCZH16, SC18, Tav12, TDOD17, TYL10, TXL10, TL15, UV18b, WWC17, WLL11, WLWT12, WWD\(^{+15}\), WHM14, WWX\(^{+11}\), XZYS10, XCL\(^{+18}\), YMY12, YXK11, YYW\(^{+12}\), ZLWZ16, ZMB\(^{+17}\), dCSD\(^{dMC}\)13, dSDPG11, dCDC\(^{+11}\), dLRR11. Beyond [Chu12, DCD11, Dob14, EAA17, ZWE12, CTVA12, MA10, RB18, SK17a, Var14, VVN16]. BGlu1 [WHS\(^{+13}\)]. BH [Kim13, XZZ\(^{+10}\), SLZ\(^{+11a}\)]. bi [MMR\(^{+10}\), MHHP\(^{R}\)R\(^{+17}\)].


Bimolecular [LQ13, DAA16, WLWL14]. binary [AD17, CLL\(^{+11}\), GE12a, Kan18, LMC19, MS14b, RKCK19]. Binding [ESLM19, GB18, RWW\(^{+19}\), ZFW\(^{+13}\), ATS\(^{+11}\), BLB18, BBM17, BJ17, CSDK\(^{+12}\), DPK18, DTF\(^{+11}\), EKN10, FFhC11, GM11, GGD12, KKM\(^{+12}\), KB19, LCT14, LNI12, MS14a, MZB16, MPTR12, MS14c, OT14, PKS\(^{+16}\), PP14, SH19, SAHA12, Shi13, SKB18, SW12, SJW13, VBK18, WTH\(^{+11}\), WDJ\(^{+17}\), XL11, dCSD\(^{dMC}\)13]. Binuclear [RALK18, SS19a, WLS\(^{+19}\), ZLY14].

Biochemistry [AM13a, KRH13, KyH13a, KGK13, LSR\(^{+13}\), OM13b, PKS\(^{+13}\), PPK\(^{+13}\), SKHN13, Shi13, TYN13, XTLA13, YIY\(^{+13}\), YIY\(^{+13}\)]. biodiesel [MCRS16]. bioenergetics [Blo15]. biogenic [MBTVR12]. bioinformatics [RNP13].

Bioinorganic [BBA16]. biological [Bra11a, CWL\(^{+13}\), CAPGAIG18, Chu12, LB14a, MG12, MMP11, XHZZXZ10]. biologically [ASHF13, KM12b, KSD10, VO11]. bioluminescence [CYLL11].

Biomimetic [ADR\(^{+18}\), WRW\(^{+18}\), ZSHL16]. biomolecular [Mit11b, SKV12]. biomolecules [BMTT11, Dnm12, IKS08, IKS10]. biophysical [WSV10].

Biophysics [AM13a, KRH13, KyH13a, KGK13, LSR\(^{+13}\), OM13b, PKS\(^{+13}\), PPK\(^{+13}\), SKHN13, Shi13, TYN13, XTLA13, YIY\(^{+13}\), YIY\(^{+13}\)]. biorelated [LGZC15]. bionautical [BVP14]. bipartition [Du12]. Biphenyl [JMX\(^{+15}\), BMF13, RS11b]. bipolar [RS11b, Shi14]. bipolaron [PDm13]. bipyramid [SALK19]. bipyridine [LKZ\(^{+16}\)]. bipyridine-ligated [LKZ\(^{+16}\)]. biradical [KMK\(^{+16}\), KMM\(^{+18}\), KSN\(^{+10}\), KYH\(^{+13b}\), ZZW11]. bird [WLZ18]. birefringences [RC11].

Bis [BSM\(^{+15}\), Jac12, LYY11, LWJL10, LZZ\(^{+17}\), MCC13b, Pli18, RNDA\(^{+10}\), SDR\(^{+13}\), SAHAA16, QZCJ10, QZXP17, dARAV12, JWG\(^{+12}\)]. bis-actinyl [QZXP17]. bis-azopyrroles [Jac12]. bis-dithiolene [SDR\(^{+13}\)].

bis-furylfugimide [LZZ\(^{+17}\)]. bis-heterocyclic [LWL10]. Bis-imino [BSM\(^{+15}\)]. bis-tert-alcohol-functionalized [Pli18]. bisadduct [LYS\(^{+19}\)]. biss-cycloheptatrienyl [ZFC\(^{+17}\)].

bisimide [JR19]. bismuth [MS14b, MHHPR+17, MLK17]. bisphenol [BLWJ17]. bisphenol-F [BLWJ17]. bisphenols [SN11]. bisphospho [SLA12]. Bistability [SS19a]. bit [Ish14]. bithiazole [SAHAA16]. bithiazoline [Qu13]. BiVO [DWX+16]. Björn [Pyy11, SA11b, Sha11b, SL11]. block [GDM+10, JHL+18, KS19, MAA10]. block-copolymer [GDM+10]. blockade [ZX12]. blocks [LLZ+14, Sza13, XWP+18]. blue [Kry10, LXW+14, SLS+14, SHW+13, TU10, dOR10]. blue-emitting [SHW+13]. blue-green [SLS+14]. blue-shifted [Kry10]. blue-shifting [dOR10]. BN [LGHL11, BSS15, FKL+12, GLT13]. BnHn2 [LCZ15]. BnHn2- [LCZ15]. bodipy [TPT19]. body [ARG11, BSO16, DLP17, Fri12, GR11, Hog13, IM15, KRG+13, LV12, Lin14, Lya14, Per10a, RAN18, RAGM10, SK17b, SIB+13, SHKS15, Zak16]. body-fixed [IM15]. Bond [CP13, FC19, GRLA18, HS15, Mar11, MPMCM+11, RL12, SB10b, ZZZ12, ZFC12, dFR15a, AV19, AGB19, ABKJ18, AD17, AG19, ASK15, AMMB+18, BCP10, Bla15, Bou12b, BWB+18, CC11a, Che12, CYC+15, Coo12, CF17, DL17, EKN10, EMS16, FGD+19, FKC12, GIO12, GI11b, Gi10, GWE18, GPM+15, GZBH18, HNH+12, HHL12a, HHL14, HAX+18, JLG+12, JE10, Kal18, KZA+17, Kan18, KK14a, KK11a, KM12c, KN15, Kuz19, LZZ+11, LW18, LW15, MNV+17, MTR+19, MGB18, MBSMC18, MBA+19, MML11b, ND11, Nal12, NHB12, NRS11, NR1+11, NRHJ11, OKR12, OK16, OHDA13, PCMG12, PCK19, RJA+10, RI19, RB11b, RKCK19, SIS10, SSK+12, SH18b, Sch10b, Sch13, SMEH16, SRA+11, SCL19, SBD18, SC18, TL15, Tob19, TCA10, VVJ15, WCGD12, WTW+15, WLC+17, XHZXXZ10, XX12, XCD18, YYY+13]. bonding [YL10, YS18, YZZ16, ZAE10, ZZX10, ZCC11, ZYL+14, dFR15b, dSNBG08, LCM+11]. Bond-dissociation [SB10b]. Bond-extended [MPMCM+11]. bonded [CdLdSC18, CCP18, DLM12, DMBL16, DB15, GCD13, IKS08, IKS10, KS18, LJ+11, LJW+11, MT10, Mit11a, MS14c, OA13, RNE10, SGK12, SPI14, ZLZ+14, ZFS+11, dSCC12]. Bonding [Con10, Mil12, TFMC19, XWC11a, ZPR10, ABM+19, AMK10, AG19, BHA19, BMX+19, BG11b, Buc10, CLXZ12, CPF12, CG12, CCL+16, Cha10, CNSK11, DMS+10, DB15, EPS+16, EAV16, Fin14b, FC19, GI14, GLXL18, Gin10, GORW19, GPM+15, HSYM11, HYD11, J113, KK13, KdPNS16, Kry10, KM19, LRY+17, LFP+19, LWL19, LW18, LBV16, LYD+18, MCCGM+19, MS14a, MPD+15, MT10, MC12, MKM11, NZLG15, NE11, Pan16, PK13b, RY+10, riv11, RCS10, SM19, SJZ+18, SYY16, SCI8, UDVT10, WSML16, WJ11, XYZ10, YZW15b, YRN+11, ZFC+17, dOdCMUdALR11, CF18, GAPK+19a]. Bonding/ [CFV18]. bonding/antibonding [CCL+16]. bondons [PO15]. bonds [ABS13, AKHS13, AM18, ALHC18, BLR12, BL11, CG12, CDL+19, DR18, DLM12, DLLA10, ED16, EEMSS14, HB14, IROW10, JLZ+17, KKC14, KKG12, LLF+12, LLG+12, LZD+11, LLZ+12, MK11, MK12, MAT19, MJ16b, MGB18, MB15, NBL12, NZ13, OS10b, PRFR17, RRVJ10, Ril10, SSI+10, SSK+12, Sch13, SMP10, SIS+08, SPI14, SS11, SM14a, SW12, SCZH16,
C [AM18, Ban12, BDF+18, BCP10, BGFD14, BBYZ18, yBZfC18, CJMC19, DQZF12, GWM11, GZW16, GB13, GCD13, JLL+18, JLG+12, Kal18, Kl12, Kn15, LKN13, LCS+11a, MLY+16, MGD11, NBL12, OGvSG18, PAKA15, PP14, SUL+11, USL+13, VF13a, VLK+11, WLZ+12a, WLZ+12b, WZW17, WSL+11, YK11, YZL+10, YLZ+17, YL11, ZQJW13, ZHL+19, ZW15, ZLWZ16, ZCTG18, TSKN12, YB11, BHA19, yBZfC18, CCEGK12, CWL+13, CRSB12, CTDLA10, DFK16, DSFT17, EML+11, FBRBR12, FBO+11, GB13, HV11, HLB19, HHL+12b, IMS+13, JB18, JCCZ12, KWC10, KZA+17, Kan11, Kl11b, KK12a, Kl12, LCL+10a, LBY+14, LZW+15, LCZ15, LD13, LDAA+11, MNP+11, MS11, MS17, MPFGS19, MC18a, NL11, NMIP14, Nik11, OCL+18, PTS+11, PAKA15, RR11, RRCO11, S¸ BAT16, Sat11b, Srt19, SCTW10, SW12, SZY17, TG13, TSKK17, WCTR+13], C [WZW17, WWGW18, XCY15, XCD18, XZG+18, YS18, ZPM10, ZLWL16, ZJC+13, DZO12b], C-H [YS18], C1s [LdBF+12], C2h [KS18], C60 [DI10, GHGF12], C=S [JLG+12, JLG+12], Ca [VO12, WCY+10, YLW+13, CRB+12, DTEMK11, GR11, MPD+10, MPTZ13, SBB16, VPFD10, YYI+13], Caballol [dGR14], CACA [Ser11a], cacao [dAGNJT12], CaCuO [Fuk12], caffeine [LCG12, PRG+10, ST15, PRG+10], cage [yBZfC18, CS13, DI18, GAPK+19b, JL12a, SL10, WLZ+12a, KK12a], cage-like [JL12a], caged [PAKA15], cages [NW12, XYL+18], calcite [SC11], calcium [Ish14, RCGLV+14], calcium-doped [RCGLV+14], calculate [ZLE17], Calculated [SPO+11, Dw13, FKL+12, 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, BBYZ18, Boe12, CP10, DK13, FLCHL10, FBM+10, FS16, GWZ+14a, GCDNGS12, HM1+15, Han19, IK18, KMK+16, KHH10, Kni13, ILBqD+19, LIK15, LSKM19, MGK+12, Mum13, MA12, MIt11c, dMOB12, PS10a, Per10b, PCR+11, Rit12b, SBM16, SMGZF19, ST15, SRASZ16, TTT13, VF13a, WZH131, XCD18, YK13, YM14, YHI14b, YLYC18].
calculational [SC12a], Calculations [KH10, KV11, LKL13, SR19, TWHZ14, dHLds12, AV19, AK17, AFA13, ADB10, ACMRN10, AGG+18, BCK19, Bas11, BB10, Boul12, BJ12, Buc11b, Bud12, COCF+14, CK17, CSTA16, CFÖ11, Dau16, DSL15, DAE+12, DWX+16, DZO12c, DZO12a, DFF+13, ESS13, Eng16, FSK+11, GAPK+19b, GVPC10, GsaY11, GFZ13, Ghu13, GJ18, GE12b, HK11, HHCA10, HH18, HS1b, HL19, HNBS18, HZS14, IKC18, JH13, KAR12a, KKL14a, KG17, KRK+17, KPCV18, KSS12, Kim13, KJ15, KJ16a, KJ16b, Kim13, KYH+13b, KPH+12, KK12G, LRP+11, Leh19a, Leh19b, Leh19c, LCL+10a, LC16, LY+19, LCK+16, LLZ+12, LNI12, MCCGM+19, MJ16a, MWC13, Mit11b, MIt11a, MFLP12, MSY+12, MPT11, MPTZ13, MJ19, NS19, NKWT19, NMS14, NZLG15, yOFTH15, OKK10, OCGM+19, OPP+14, OH19, OSJ+12, Pan19, PP19a, PK16, PBR18, PB10, RS12a], calculations
CASPT2 [BDFM10, BDR12, ČFČ11, GLOGM+11, KZZ13a, LCL+11, LGP+12, MR11, Pul11, RS12b, SKTI15, SZZ+12].

CASPT2//CASSCF [GLOGM+11].

CASSCF [BDFM10, DAR+11, GLOGM+11, Lar11, Ols11a, PE11, RS12b, RSN12, SZZ+12, SBL11].

CASSCF/CASPT2 [SZZ+12, BDFM10].

CASSCF/MRCI [DAR+11].

Catacondensed [RB08, RB11a].

catalysed [SMRK18, ZYSW17].

catalysis [BvWG14, KJ14, MMM+12, MCRS16, PIS18, Sic16, SLS+15, XDM+10].

catalyst [ENV15, Esr18, EM19, GB18, Hög13, JXX+15, LCM+11, TM19, Var14, ZQW+17, ZBG+19].

catalyst-free [ZBG+19].

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

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

catalyze [XGH18a].

catalyzed [AKC10, AZD+11, CAPGAIG18, CWZ+10, Che12, GCZ+14, HZZ+19, JL12b, JXQ15, LCM+11, TM19, Var14, ZQW+17, ZBG+19].

catalyst [ENV15, Esr18, EM19, GB18, Hög13, JXX+15, LCM+11, TM19, Var14, ZQW+17, ZBG+19].

Cation [ZLWZ16, ATS+11, Ber13a, BMX+19, DW11, ESR13a, GYY+19, HZZ+19, JL12b, JXQ15, LCM+11, TM19, Var14, ZQW+17, ZBG+19].

cation [ZLWZ16, ATS+11, Ber13a, BMX+19, DW11, ESR13a, GYY+19, HZZ+19, JL12b, JXQ15, LCM+11, TM19, Var14, ZQW+17, ZBG+19].

cation-exchange [PDR+14].

cation-exchanged [PvS10].

cationic [BCGC12, FTB11, ZQJW13].

cations [BMF13, ESLM19, GK12, HFA+19, IGMK11, LGP+11, LPG+12, MMR+10, MKM11, NKWT19, PDR+14, SHE10, WLWT12, YLW+13, ZLWZ16].

caused [HYH+10].

causes [ABP13, MFM18].

causing [MFR10].

Cation [ZLWZ16, ATS+11, Ber13a, BMX+19, DW11, ESR13a, GYY+19, HZZ+19, JL12b, JXQ15, LCM+11, TM19, Var14, ZQW+17, ZBG+19].

cave [XGH18a].

cavities [MGK19, Pup11a].

cavity [PCR+11, OPC17, RAFFF18b, RAFFF18a].

CBr [WZHZ13].

CBS [CFOC+10, VF13a].

CBS-Q [VF13a].

CBS-QB3 [CFOC+10].

cc-pV5Z [SLS+11].

CCl [EMS16, LZZ+11].

CCI [SKS11, LGW11].

CCSD [CK13, VV13, BL12, CPF+11, DVP18, JdOS16, SLS+11, TD19, VV12].

CD [SZY17, ASHF13, ZZZ+10, XWCI11a, LKLW11, XWCI11a].

CDO [ADR+18, SAHG11].

Ce [WLG+11, WSL+11].

cefotaxime [LBMI11].

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

Cell-penetrating [KMT+12].

cells [AGJ12, BDG17, FFDP16, FM16, cLqFtW+14, LYS+19, MY17, PMAP12, SG19, Tz11, ZAP11, Zha17].

Cellular [Kuv10].

cel lulose [FBKB17].

Center [Buc10, Buc11a, CRSB12, CN12, Hog10, HZS14, Koc13a, MNPN18, Ta11, Yam10, YD17].

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

Centers [ASD14, YG11a].

centrifugal [CLXD15, IIH16, ZLJ11].

centrosymmetric [KPT+17].

Century [Pup11b].

CeO [QCB+10].

Ceria [KJ14].

Cerium [CCA+12].

Cesium [MMR+10].

CF [IAW14, Mor11, Mor11].

CFC [dOdCMUdALR11].

CFP [KyH13a].

CGR
ASMP15, AD17, AMMB+18, BF11, Bal16, BL10, BL11, BG11b, Brä13, BVRM10, CJBBMMAPR19, CKL16, CLXD15, CFGC11, CPAT11, DKZ+10, DPK18, DSL15, DPRK12, DFK16, DMS+10, DLM+11, DMLB16, DSYT17, EAK+10b, EML+11, EMED+12, EMEDP15, FBO+11, FBD+13, Gag11, GP13a, GRCGRRHT19, GFPVAV19, GA19, GI11a, GhZA10, Gru17, HMA+19, Hop15, HAX+18, JN13, KWC10, Kal18, KBGIC12, KMK+16, KM12c, KUTS10, KK11d, LZZ12, LYT+17, LI17, MC11a, MPE15, MTR+19, MC14, MG12, MQ17, MKM11, MBT+12, MML11b, MPG16, NC11, Na12, NZ13, Ném14, NVPIC+13, NRP+11, NJA+12, OSI10b, OWD18, OSJ+12, OEDB11, PWY+18, PO15, Qu13, RLW+13, RGTS11, RNE10. **chemical** [RMP+14, RR19, RBTL19, SSI+10, SSK+12, SAG13, SBEH11, SKHN13, SC12a, SW10, SN15, SM19, SC10a, She14, Sh13, SIS+08, SKM11, SR13, Sko16, SFY12, SBKJ18, SRA+11, SK10, SSB+12b, TFBG14, TYN13, Tmp15, TMC18, TSTC17, UTTN13, UJSJ13, VOK+18, VO11, VO12, WYM15, WLD+10, WLWL14, YNL18, YSS+10, YYI+13, YB11, ZBK15, ZC12, dHLD12, vL13, vLRRK15]. **chemiexcitation** [dSM19a].

**Chemiluminescence** [dSDi13b]. **Chemisorption** [OD16]. **chemistry** [Vie17]. **Chemistry** [AH19, ÁIGVZ12, Brä13, Hog13, IFT13, KYS13, KYH+13b, TBRIS12, ZIS13, Ban12, Bar16, BMRM19, BZBZ13, Blo15, BHH+13, BT15, Buc12b, Cav13, CA1916, C16, C14, DC12, Gall11, GGZZ16, HR13, HEVMSA+19, IK14, Jia15, Kap12, Kar09, Kar10, KC19b, KN15, LSR+10a, LSR+11, LJ16, LF5+11, LCZL15, LSKM19, Luz11a, MML+16, MEF+15, MMCMV19, MQG13, MPGGS19, Mor13, NBZG16, NTCK13, Nic11, Nic14, NMSR14, OM13b, PTH11, Pup11b, Puz11, Rei15, RNB+10, SDP+16, She13, SG14, SPM+15, Tch16, TBB+19, TBRIS10, TBRIS11, Tri14, TB15, VYN+16, VMM11, VBJK18, WYWL13, WWX+11, WR14b, YZ13, ZWL13, ZWSF16, DC10, SG14, BT17, Tch13]. **Chemists** [RA10b]. **chemogenomics** [IAK13]. **chemometric** [LSR+10a, LSR+11]. **chemosensor** [LWZ+14]. **CHF** [STL12]. **Chiral** [YWR+18, BtTG11, CPL15, KGVI11, LPM+11, LMCZ11, LW13, QCW+12, SFW12, WTW+11, YYW+12, ZSS+13]. **chirality** [Luz11b, SD13a]. **chiroptical** [Cap16]. **chirp** [GRLA18]. **CHITEL** [RA10b]. **chloramine** [SZL+15]. **chloride** [EHDK11, EKD12, MM+12, SK11, dOLdV13]. **chlorides** [BLM+12, HSN+11]. **chlorinated** [FBO+11, KZA+17]. **chlorine** [DGX12, cLqF1W+14, MOY13, XXB+X+13]. **chlorins** [CJSLN11]. **chloro** [DDC+12, DPRK12, PSK19]. **chloroalkenes** [MLB+12]. **chloroanilines** [HLZ+14]. **chlorobenzaldehyde** [SRA+11]. **chlorobenzene** [SGL19, SC18]. **chlorobenzofuran** [ASMP15]. **chloroethyle** [CZJZ12]. **chloroethynitrosoreses** [ZMZ13]. **chlorophenol** [ASW13]. **chlorophenyl** [OEDB11]. **chloroquine** [KdPNS16]. **chlorotrifluoroethylene** [OCB+10]. **CHN** [RB11b]. **CHNC** [DW12]. **CHO** [DZ11a, Sch10b]. **choice** [AGP13, FSB16]. **Cholesky** [BVA+14, CPF+11]. **Choosing** [KBJ17]. **Chou** [QZH13]. **chromates** [Zen11]. **chromium** [HM12]. **chromogens** [JA12]. **chromophore** [BF11, BSM+15, GLOGM+11, LORR+12, TCM+12].
TW10, TFMC19, TPCJ+12, UKF+11, VSMK13, WJL+11, WCS+13]
custers [WJL+10, XGH1a, XWC11a, XWC11b, XF19, YSK+12, YGLL10, YZZ15b, YJ17, YZ12, YC13, ZWSF16, ZRR+11, ZCW16, ZCP11].
custers-continuum [DQZF12].
[EMSB15, LZZ+11, Oui12, ZLWZ16, CP10]. CNaY [LZZ+11]. CNC [Zha10].
CNH [Tap15]. CO
[BGFD14, BAA+18, BDR12, DPDR11, DWPK14, GGJD13, WZC+12, WRW+18, Kim19, VD13, YL11, BD14, BGFD14, BLdV19, CRSB12, CCS13, Esr18, EM19, FTB11, GSB10, HDC+11, LCT14, LW+18, MPM15, MMP+18b, RDB18, RDB19, RBTL19, SCLCPB12, SAHA12, SLSZ13, Sri18, Sri19, SCL18, WZC+12, YGLL10, AAA12, CRB+12, GZMC11, Kim18, MRT11, NKWT19, ZYSW17, WRW+18]. Co- [GZMC11]. Co-based [Kim18]. CO-photolysis [BGFD14]. CO/ [WRW+18]. Co/Ni [AAA12].
Collective [MLDP10, BM10]. collinear [SABA+12]. Collins [Sit15].
collision [LWWZ13, LPM+11, MGK+11, SABA+12]. collisions [BMTT11, BHV+11, DSC+11, dDGMB10, LdAA+11]. comb [MPC10].
Combination [KYH+13b, SN15, Buc10, CK13, DQZF12, SZZ+10, SLZ+11c, SLS+11, VV12, VV13]. combinations [Boe12]. combine [Lin14].
Combined [IK18, SJZL12, TAY11, KP11, MLDP10, NZ13, Tan13, ZLWY13, BBB+12b]. combines [WZX15b]. Combining [PC16]. combustion [MPGGS19].
CoMFA [MGK+12]. Comment [BR16, CK13, Cin20, COP16, FKBG19, Fer19, HS15, KBG17, Lad14, Lui13a, Man16, MBSA16b, MMB20, PS14, Tour13, VUC13, dSSF16a, dFR15a, HYZ19, PS13b, VV13, XT1A14].
commentary [Ols11a]. comments [Br11b]. commercial [FT15].
Common [VSL+15, ESLM19, LCH14]. compact [LQZZ12, LLZ14].
compactification [DTF+11]. Comparative [BLRdA+10, BO11, CLH14, DTEMK11, FDG18, LJJ+11, LL19, LL17, MF+13, NS2a, PI13, SD16a, dAGNJT12, CCB+12, FFF10, HNN+12, KMI12a, KKM+12, LCT10, LLZ10, ONBP11, PRUP+13, RS11b, YL13, YZ14, YLZ+14, dSSPG11].
comparing [HXDY16]. Comparison [AM13a, BPT12, CDSK12, Han19, JdOS16, MR11, RALK18, SSP+17b, SM13, UV18b, YF16, ZHL+19, ABL11, BLL+13, BGK16, CCI9, GP13a, HDQ+13, Kan11, KC16, LdBF+12, LFZ13, OKR12, dSMRFS18, SD13a, Sch13, SG19, SBK18,

Complex-scaling [JH13]. complex-valued [YW16]. complementant [XWCY11]. Complexation [ESLM19, SHE10, ZKKR11, ZAE10]. Complexes [ALMY18, GHGF12, AC19, ADR$^+$18, AM18, BHMN19, BPG$^+$10, BAP12, BHA19, BZBZ13, BLdV19, BPK19, BCS$^+$12, BB16, BS12, CRB$^+$12, CPF12, CTW12, Con10, CLMY12, CADSG18, DSD18, Den19, DPDR11, DG19, DCdG10, DD$^+$11, ED16, ESS13, EMSB15, EMS16, FBWR12, For12, FBD$^+$13, HS11b, HL19, HYD11, HZZW11, JW19, KRK$^+$17, KV11, Kry12c, KBMM10, LJL$^+$11, LYW11, LXW$^+$14, LYR$^+$17, LYL$^+$12, LSD13, Lu10, MZB$^+$13, MCE11, MNV$^+$17, MC17, MGK19, MI18, MI19, MG12, MKM11, MS14c, MPRCEG12, ND11, NFD$^+$10, OAC17, OPP$^+$14, OVT$^+$16, Owe17, PM17, PRG$^+$10, PAKA15, RFFGPP$^+$16, RB11b, SS10, SVRGV12, SG19, SGKG12, SRASZ16, SAHA12, SLS$^+$14, SK11, SS$^+$17b, SPI14, SHW$^+$13, SM17, SK12b, SS13, TTD13, TMM$^+$14, TL15, UDVD10, VO12, WLS$^+$19, WXW$^+$11, WZW17, WHM14, Wu11].

VPGC12, WCY+10, WWQG17, WLL19, YLWrL12, ZFC+17].

Comprehensive [LKN13, RYM12, WJY15, BTH18, FKC12, KI15, SL10].

Compressed [Man16, MBSAG16a, MBSAG16b, SBM16].

Computation [SPR19].

Compton [Kar12c, Kar15].

Computation [AM13a, AH19, AMK10, BYAT13, BGJSM+18, BJ17, BBA+16, BCS+12, CAA19, CSHK12, CLY12, CTH14, EM17, EBH11, FFP16, For17a, FNIT16, FR10, WKE17, Zen11, GI11c].

Computation [Man16, MBSAG16a, MBSAG16b, SBM16].

Compression [MNS10, Oni10].

Concentration [BS16, HMB16, IKN13, RTG+19].

Conceived [AF19b, GCK+17, Mak15].

Condensed [AF19b, GCK+17, Mak15].

Condensation [Chu12].

Concurrent [EMED+12].

Condensate [DCC11].

Conformation [RRCO11, Ali19b, BEM11, CGG18, CP16, DVDBM11, GBK18, HFD11,
JH15, KUY16, Luz08, NVI10, PBR18, SYL+18, Sha11b, SLZ+11c, SWS12, SZL+14, TG16, VVVB10, YKN13, ZST+10. configuration-interaction [JH15]. configurations [Buc12b, FM16, RSN12]. confined

[ATL+14, BChNH16, BJ12, CAAI12, CCP18, CFGC11, CSP+10, CDT12, CGIAI12, CJOW11, Cyhi11, DCOC+19, KP10, Kin13, LJSS12, MPTZ13, NH18, NB17, dMOB12, Per10b, RKR16, SGB11, SYL+18, SLZ+11b, SXS+12, SLS+12, SS12, SM10b, SWS12, UV18b, VLFG12, VO11, WZH13, Wit18]. constituent [MKHN11]. constrained [Lev10, SS12a, WCM14]. constrained-search [Lev10]. constraint [PSMD16]. constraints [CM16, Fin17, MB12, Oh13]. Constructing [Beh15, KFY+12]. construction [Pop15, SX15, WR14a, MPB11, RVO+14]. Contact [LJK+18, DK13, XYS10]. contacts [EAA17, GI14]. containing

[Con10, DLLA10, FBU+11, HZG12, LWJL10, MPD+15, MB15, NCMC+18, NFD+10, NFQ+11, RRR16, RRR19, SM12, SGT10, YGLL10, YZZ16]. contamination [Bla15, GXZ+14]. content [ALRA10, Sha11a, TRZ+19]. context [BBM17]. continuation [RW11]. continuous

[Ale13, Ban12, Mor13]. Continuum [AF19b, JCC10, Cam10, Cam12, Cap16, Car19, COCF+14, CML+16, DZ012c, DQZF12, FRGC10, GMA+19, Kit15, Li15, LSKM19, PCR+11, RTG+19, RFE18+16, SL10, SLS+19, WML11].
EAK\textsuperscript{+}10b, EAK\textsuperscript{+}10a, EI11, THSR13). corrosion-inhibition [THSR13].
cosine [GH11, GE12b, LLH15]. Coulomb
[SS12, CF14, ARG11, BPL13, BBL12, Fin16b, FRGC10, Fuki12, GH11, I0O18,
JH13, KH12, KWWH18, KK13, LLH15, Luz12, Nag16b, NDP10, PGGRMP10,
Rit12b, Roy13, Roy16, SMD11, Sil14, TC12, WWGW18, ZK12].
Coulomb-attenuated [NDP10]. coulomb-attenuating [CF14].
Coulomb-like [PGGRMP10]. Coulombic [Roy15, YW11b].
Coulombic-like [YW11b]. coumarin [MNP19, MDND0\textsuperscript{+}16]. coumarins
[GTSC\textsuperscript{+}19]. Counter [XPGA12, ZLWL16, MMSC19, Oni10]. Counter-ion
[XPGA12]. counterpoise [KPH\textsuperscript{+}12]. counting
[JJL12a]. Coupled [BJ12, Cam10, Cam12, Car19, PCV19, Sto18, VVKB10,
WYC17, BVP13, BVP14, BSMT\textsuperscript{+}15, CSVCB12, DMB12, DML12, LRP\textsuperscript{+}11,
LP10b, Luz08, MPT11, PB10, RS12b, RSN12, SZH\textsuperscript{+}10, Sza13, Tob19, Var11,
XDM\textsuperscript{+}10, YK13, ZE18]. Coupled-cluster
[Cam10, Cam12, PCV19, LP10b, PB10, SZH\textsuperscript{+}10, Sza13]. coupling
[ATL\textsuperscript{+}14, Ash18, BJ12, BSVT12, CCP18, CFG11, CSP\textsuperscript{+}10, CDT12,
IROW10, Kry10, Lar10, LKOS17, LW15, MKD19, MC18b, PM12, RCP14,
SSI\textsuperscript{+}10, Shi18, SHS\textsuperscript{+}13, WTP\textsuperscript{+}19, Wtt18, YSS\textsuperscript{+}10, YH14b, ZLS\textsuperscript{+}18].
couplings [HKWL13, Kax15, LB19]. course [HSYM11]. covalency
[MML11b]. covalent [ABS13, AB16a, MURR13, NE11, YLH\textsuperscript{+}19, 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, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14t,
Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z, Ano15a, Ano15b, Ano15c,
Ano15d, Ano15e, Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l,
Ano15m, Ano15n, Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u,
Ano15v, Ano15w, Ano15x, Ano15y, Ano15z, Ano15a, Ano15b, Ano15c, Ano15d,
Ano15e, Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m,
Ano15n, Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15v,
Ano15w, Ano15x, Ano15y, Ano15z, Ano15a, Ano15b, Ano15c, Ano15d, Ano15e,
Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n,
Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15v, Ano15w,
Ano15x, Ano15y, Ano15z, Ano15a, Ano15b, Ano15c, Ano15d, Ano15e, Ano15f,
Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o,
Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15v, Ano15w, Ano15x,
Ano15y, Ano15z, Ano15a, Ano15b, Ano15c, Ano15d, Ano15e, Ano15f, Ano15g,
[LQZZ12, MPT11, MPTZ13, LLZaH14]. curved [DI18]. curves
[DHZS11, GM11, PPDF11, SAS+12, Vik11b]. cusp [RLER14]. CuT1
[VLG12]. cutoff [KdSM+10]. cutting [LCK+16]. CX [LGW11]. cyanates
[KL0S17]. cyanide [CMCN11, DR18, GWZ16, WWLZ17, ZW15]. cyanins
[ESLM19]. cyano [KPL+17, RS11b]. Cyanoacetaldehyde [KS19].
cyanobenzenes [EMK14]. cyanogen [BMBD10]. cyanospherands
[ELC08]. cyano [VGL12]. cutoff [KdSM+10]. cutting [LCK+16].
cyclacene [OCGM+19]. cyclacenes [BLB+18]. cycle [KB13]. cycles
[BvWG14, COCF+14, Sic16]. cyclic [ABM+19, BBK16, DGA+13, FJK14, GHGF12, HL19, Jan10, JB18, LMCZ11, Luz11a, MZLM17, MWH+13, OB19, QTCL10, SB16, XZG+18, Con10]. cyclization [ALMY18, KSAK17, LD17]. cycloaddition
[ABM+19, BL11, CJGTL12, DI10, KI15, LLF17, LFTL18, LCS+11a, LXLL11, NAK+17, SKTI15, WLWT12, YNLD18, ZRGE+19, ZWWY10].
cycloalkanes [DFV+12]. cycloalkanone [HZZ+19]. cyclobutadiene
[LX13, ND10]. cyclobutane [LSL+08]. cyclobutene [QB15]. cyclobutyl
[DCY12, SC12a, SC12b]. cyclodextrin [NMHPVG12, SRVGRG12].
cyclodextrins [PEA+12]. cyclododecane [DFV+12, SAS+12]. cyclohexa
[KAOB11]. cyclohexadiene [TXK+19, ZWWY10]. cyclohexane
[WWGW18]. cyclohexyl [CZJZ12]. cyclohexyltitanium [GMM+18].
cyclohexadiene [LXD13, ND10]. cyclohexene [KAOB11]. cyclopentadiene
[CRI11]. cyclopentane-1 [OPP+14]. cyclopentane [OPP+14]. cyclopentane-1 [OPP+14].
cyclopentanone [PCR+11]. cyclopentene [ALMY18]. cyclopentenols
[VOK+18]. cyclopentene [ALMY18]. cyclopentene [ALMY18]. cyclopentane
[TBA+13]. cyclopropene [CT14]. cyclotetrazenes [FST19]. cyclopropane
e [DFV+12]. Cyclodecane [DFV+12]. cylindrical [D+16]. Cys
[ScBR+10]. Cys-Asn-Ser [ScBSR+10]. cysteinate [WHM+14]. cysteinate
[AED+18]. cysteine
[ASD18, CLMY12, HYD11, SKS10, YWH+12c, dAGNJT12]. cysteine-Ca
[CLMY12]. cysteine-formaldehyde [YWH+12c]. cysteine-thymine
[HYD11]. cytochrome [RD+11, TSKN12]. cytosine
[CTYA12, Cyb11, JS18, KUS19, YM13].

D [IIS+17, Kan11, STL12, SYZ17, TSL11, XLLZ10, ZGSM15, CC11a, ÖEB11, BEM12, BMX+19, BAB+18, DLRMFY10, HGB08, KHI10, KSO19, LCM+10a, LQZZ12, LLZA+H14, NF11, OD12, PTD+12, QTCL10, SLA12, SSS15, SK10, VY18, WTH+11, YGLL10, YSW11, ZHI12, CYS11]. D-
[SSS15]. D-dimensional [DLRMFY10]. D-wave [KHI10]. D3 [SSB19, SA18].
DABA [Ser11a]. DABCO [LLF17, LD17]. DABCO- [LLF17].
DABCO-catalyzed [LD17]. damage
[CAPGAIG18, FMP+17, POLV12, SS18a]. dance [FK18]. Darmstadtium
[DR18]. data [CFV18, EKN10, LLH15, OKR12, SAG13, SDP+16, SMEH15, SBKJ18, VLG12]. data-base [SMEH15]. database [TBST10]. dataset


decanethiol [FFF10]. decapeptide [DGA13].
decarboxylation [EAH13]. Decay [AC11, ASD14, Cao17, CCM08]. Decisive [SC18].
dehydrogenation [HSYM11, NTN10, WZ13]. Delayed [SGG10, GM18]. Deletion [Cin11a]. delivery [RdPW12].
Delocalization [DZO11, LNI12, ARH13, AT18, LDKB15, MJ16b, NE11, NRGS11, RBVAG18, WDSL14, WWD15]. delocalized [ALK18, DG19, Joh17]. delta [DAC11]. demon [CD15]. denaturation [BMB12]. Deng [Roy14]. denoising [SRMB15]. denominators [CPF11]. dense [BN12, DW12, Ng12]. densities [ALRA10, ALRA11, BPL13, Fin15, LS17, MAT19, MT11, MNZP19, SS19b, WGL10, ZL12]. Density [Ano13-49, BHA19, BGBV12, BJdIAM12, CCL13, CM12, CD12, DCBB11, DSZB18, DQZF12, EM16, ED16, FZ18, GMR18, GGD12, H12+z14, HK11W13, HY11, IS13, IN13, JS17, Kar13, KCC13, KK14b, KSA17, Kt14, Kt17, L14, LW14, LWX14, LBY14, MLC11, MW16, MUNZV12, MIN13, MLB12, MM13, MCRS16, MOH12, NTN10, NZAV10, PS10b, PS14, PMH16, RGPZ13, SA18, SRVG12, SKY13, SS13, TOS12, Tan12, Tin13, TDOD17, TFZ15, UMS13, VUC13, WJ11, Wit18, YKM15, YL11, ZCZ16, ZRR11, dCSDdMC13, AC19, ABLT11, AK17, AM13b, AB18, ATM17, AGPDZ13, AST16, BMK14, BD14, BGC12, BVCAP12, BL19, BDF16, BDF18, BLdV19, BLKB11, CDSK12, CEFMK12, CM15, CNSK11, CH17, CZL17, CLH14, CC19, CK17, CF14, CC11b, CSTA16, DWJ11, DKS11, DPK12, DW12]. density [Dil13, DZ11a, DGR16, DG19, FO10, FDNR10, Fin16a, Fin17, FA17,


FSB16, GFP AV19, GCK +17, GM11, GJ18, GHCMCMQ17, GWME18, GD11, GCZ +14, HMA +19, HR19, HHCA10, HZZ +19, HMH10a, HMH10b, HIIH13, HZZW11, IN15, JR12, JPP +11, Jan13, JW18, Jeo18, JW19, Jou13, KK13, KME +18, KPCV18, KJ16a, KJ16b, KKL +16, Kit15, KYLC19, KDO17, KJ14, Kri13, KFS13, KG08, KM +13, KFJ +18, Kuz19, Lat13, LPO +12, LSR10b, Leh19a, Leh19b, LW11, LC16, LSP +16, LLW +11, LCK +16, LDZG16, LNI12, MYZ +10, MLW +14, MJ16a, MFK +12, Mas10, MKSG13, MLK17, MJ11, MBBT +12, MBSMJFC18, MNS11, MKW11, MJM19, Nag15, Nag17, NAK +17, NDP10, NL11, NMIP14, NMSR14, NIT16, OD16, POLV12, PI13, PK13a, PABSK16, PP16, PTH11, PL11, PCV19, PR10b, PSMD16, PRFR17, PFDM13, Per18, PJP10].

Density [PMAP12, PI16, PC13, QHS11, RLER13a, RCM +19, RPVM10, RGT11, RAMB18, RBVAG18, Rud12, RSCS10, RLZ12, RS13, RKCK19, SS10, SLG11, SB18, SFC16, SL +18, SN12, SAHG11, SLL +18, SJJ +18, SIS +10, SDM12, SSP +17b, Srt19, SRA +11, SK12b, SX15, Tan13, TA10, TCA10, TGRP19, TLC +17, TRZ +19, UV18a, VP12C12, Vik13, VBO +15, VSL +15, WKE17, WW11, WJY15, WDJ +17, WTZ +11, WR15, XNL +14, XSLF12, FxxBhD19, XGH +18b, YLH +19, YW12a, YWH1b2, YRN +11, Yu13, YF16, ZT13, ZKRR11, ZQJC10, ZLB13, ZBG +19, ZM13, ZCNG16, ZS14, ZKW17, ZZ18, Zho18, dCGAM12, CTDOLA10, LLZ +12, Ven12].

Density-based [ZKW17].

Density-dependent [IN15].

Density-functional [SVRG12].

Density-matrix [EM16, Kit14, Kit15].

Depicting [LBdV16].

Depolarization [AEM +12].

Deposition [SAHGI1, SAHA12].

Deprotonation [CFOC +10, Kry12b, PUGSF18, Shi18, WX +11].

Depurated [Cin20, MMM16, MMO20].

Derivative [BR10, BR16, Bra10].

Derived [HSN18, BSS19, DWPK14, KG11G11, LWZ +14, TPT19, WLZ +12b].

Derivatives [ALMY18, BSS15, CML +13, CCL +16, CFV18, CWB +13, CSG14, DKZ +10, DWZZ15, DNCKS +12, EI11, FSQ +11, GTR11, GB13, HNH +12, HMA +19, HS11b, HLB19, ILBS10, JLZ +17, JB11, JFDD10, KZA +17, KKM +12, KSN +10, KKG12, LGM +18, LWL +12, LYS +19, LWY19].
LCCH10, LWH+12, LCH+11, LCS+11b, LW15, MLY+16, MNV+17, MLPT10, MDNDO+16, MBBT+12, NRHJ11, OAA19, PPK+13, QHS11, RYM12, RBZ15, RMP+14, SF13, SST011, SRMB15, TZ11, TKSK17, Val17, VV18, VMC11, VHTEG15, VBO+15, WGLX10, WLL+13, WJ11, YWR+18, ZSAP11, ZZX10, ZZR+12, ZYL+13, ZMB+17, ZFC12]. derived [CADSG18, MAN15, NH18, PAKA15]. describe [CB10, MMG15, PABSK16, Sza13]. describing [Gar08, JCC10, dGR14]. description [AB18, DVDBM11, DCFD10, DMBL16, Fer19, FGD19, GC19, HFdGC14, KO14, LORR+12, MPMMC+11, MBA+19, Nas19, NGS11, SIM14, SFL+10, TCA10, TRZ+19, ZZ18]. descriptions [PC16, PCK19]. descriptor [AKR12, FDG18, PUGSFM18]. descriptors [GI10, GI11b, GI11c, GI11e, JS18, LV19, LNV+18, Nag16b, Nal15, OPAVM18, PH12, Pog12, TFA10]. Design [FZH+18, HSS18, IIS+17, cLqFtW+14, Val17, BJ17, CAA19, DC14b, GhZA10, HM10b, LLZ+14, LZZ+17, MY17, MSM16, Ném14, Oni12, OW18, SRASZ16, SAHAA16, Sik18, SLA12, SSS15, SM18, THL+15, TK16b, VV18, WWB+14, WR14a, WR14b, XWF+14, YZZH15, YHLC15, ZFW+13, ZWZK19]. designed [NTGC19, OAA19]. designing [SSB12a, ST15]. desorption [´AFV12, FTB11, GD11]. Dess [TM19]. destructuring [KRG+13]. desulfurization [VPGC12]. detachment [DZO12a]. Detailed [Sch13, Fin14a]. Details [Lar10]. detector [BMB10]. determinant [RLZ12]. determinants [CSSK+12]. Determination [ATL+14, GI11b, GI11c, IKN13, SN12, Ali14, AGPDZ13, AST16, MLW10, PT13, Ser11b, GBK18]. determine [SFW12, Tob19]. determined [Mor12]. Determining [MGM11, AGB19, Bon17, IKN13]. detonation [LZZ+13, RGTS11, WGLX10, ZZX10, ZL12]. Detours [DB13a]. deuterium [NHB12]. deuteron [HITU16]. developed [AY15]. Developing [AV19]. Development [KSN+10, Lin14, NNSN17, SR11b, SKV12, SZ15, GEL18, Kap12, KKL+16]. developments [AMMC19, HJK14, Jor18, Mur12]. device [yBZfC18]. devices [Jan10]. dfppy [ZQJ13]. DFT [YSK+12, AEKGZ12, AFC+10, ACF+11, BVCAP12, BPVDB11, BP13, Bas11, BBZB13, BLRdA+10, BAA+18, BS14, BDR12, BAB+18, BJ12, BO11, BW13a, BW13b, BSV12, BSKP11, CRB+12, CR18, CPF12, ÇAS13, CRSB12, CW16, CCL+10, CKYR18, CKB18, CFGC11, DSCO+13, DSD18, DCDD10, DCFD10, Dw13, DAE+12, DPDR11, DP16, DdG+11, DB15, DFF+13, EG10, ESDO16, ESS13, EFO11, EO11, ES17, EM19, ESBVY12, FSQ+11, FY11, FRNM12, FPGRMGHB12, GAKP+19b, GC18, GJ18, HS11b, HFdGC14, HNBS18, HhGqZZ17, JPPA10, Jan10, JL12b, JB11, JLL11, KMS+11, KP11, KP11, Kar12b, KBF+13, KAG08, KMM+18, KG17, KI15, KKG12, KBM10, LJ13, LGM+18, Les12, Lev16, LYW11, LLP+13, LLF17, LZW+18, LTL18, LW+19, LGW11, DVMC19, LKZ+16, LGS+16, MXY18, MCP10, Mar12, MCC12, MK19, Mas10, MMP+18b]. DFT [MMC+19, MFZ+18, MCL11, MS17, MML+11a, MMY+12, MAN15, Nag16a, NEEV15, OKK10, OvGvS18, OCB+10, OCGM+19, OPP+14, OVT+16, PS10a, PTS+11, PK13a, PWL+10,
BS16, CW16, CP11, FM16, GI11e, GGP13, HGB08, JdOS16, KP10, LZZ+17, MNP19, MIKH19, TW10, TFZ+15, YŞÖ12, ZCW16, Zill14. differential [Ali14, yBZfC18, CRA+11, HVR18, Nag10]. differentiation [CW11].
difficult [KLE+19, Mar12]. difficulties [Sut12]. diffraction [ŒDB11].
dihydrolipoic [PM17]. dihydrobutyric [TM13]. dihydrolysergol [RGS+13].
diphenylamino [CRSB12]. diphénylcarbène [GLXL18].
diphyformazans [TT10]. diphenylpolyménes [MMWA11].
diphosphinito [ED16]. dipolar [BL11, DI10, ELC08, YNLD18]. dipole
[AM12, Ber13a, Ber13c, BVPI4, GFB12b, GI11a, GI11c, HK11, IMS+13,
KA11, LKJ13, MA11b, MD11, MVA19, MNS11, SS12]. dipoles [SMEH15].
Dirac [DJ12, Agb12, Bay19, BCNR18, DJ95, NF11, RW12, Rit12b, SS12].
diradical [MMF+13, NYS+10, PCK19, Sh18, YS+10]. Diradicalology
[NKF+13]. diradicals [BSM+15, CKL16, ZLS+18].
direct-potential-fit [Haj18]. Directed [DKR10, ABS13].
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Divide-and-conquer-based [SKHN13, YKN13]. divide [HS11c].
divinyl [dILAI+12]. divinylenol [FO10]. division [FDG18]. DJ [Sh13]. DJ-1
[Sh13]. DMABN [CFP+10]. DMABN-Crown4 [CFP+10].
DMABN-Crown5 [CFP+10]. DMAP [LLF17]. DMAP-catalyzed
dual-level [WWHZ13], ductile [KG17], due [ALA15, CAO18, ZSZ14], duplex [PPK+13], during [HSYM11, MNC12, MSAB19, Tob19], Duschinsky [Man13], dyads [MUNZVR12], dye [AGJ12, BDG17, ÇAS13, FM16, FSBA12, cLqFtW+14, MY17, MFB11, MANP17, PMAP12, QJ13, SG19, SSS15, WKE17, WWB+14, Zha17].
dye-aggregates [WKE17], dye-sensitized [AGJ12, FM16, cLqFtW+14, MAP12, QJ13, SSS15, WWB+14, Zha17].
dyes [AGJ12, BBM17, FM16, FBU+11, GMA+19, JPPA10, JWG+12, cLqFtW+14, MY17, Mas10, PJP10, WWB+14, ZSAP11].
Dynamic [´AFV12, DLG12, KWLS15, AM13b, Ang10, B L16, CCEGK12, CEFMK12, FKL+12, FC19, KYS13, LKJ13, MNS11, NH18, RC11, RVO+14, Tob19, TSH17, TPCJ+12, YKM+15, ZWLC12, dWLC14].
Dynamical [AFM+10, BR10, BR16, GWZ+14a, Sko16, ZZ15, EML+11, Ign11, Ign12, KMF+11, NE11, PETB18, VVY18].
Dynamics [KKH+13, LLM13, MNE+13, PPK+13, RDB18, SPRD16, SPPT15, TIN13, TM13, AS19, BM16, BBB+12b, BR15, BWB+18, CTVA12, CCC19, CW13b, Cho19, CLXD15, CAPL12, Dau16, DGR+16, DLZ11, DP11, EAH13, Fra17, FUE+12, GKS10, GVPCK10, GW18, GSPR19, HDÖS12, HXX15, HHL+12b, IKC18, JHSG18, KTI+12, Kaw15, KCC13, KSC15, Kit14, Kit15, Kit17, KF17, KUY16, LWWZ13, LC19, LPM+11, LKLW11, MAD12, MMG15, Mak15, MSH13, MDC15, MP12, MCARL11, MOE+11, MMBK12, MKD19, MMT+13, MRS15, MSK+12, MPL+11, MLB+10, MBS+18, MMP11, NTGC19, Nyn14, OHDA13, PD11, PP10, PMH+16, PI16, RSM12, RP16, Rit11, SMK+12, SIT+12, SPSA11, SMEH15, SIB+13, SHKS15, SLS+10, SKV12, SZ15, SZY17, SBL11, TK16a, TPdMB12, UTt13, Vik11a, VGS10, WWHZ13, XZJ+16, Xu16, Xu19, Yak10, Yak11, YGL+11].
dynamics [YAF+15, YT14, YINM13, YLC17, Zak16, ZPM10, ZZW11, ZGSM15, ZH15, ZCG+17, ZWL18, ZRLV10].
dynamics/quantum [BBB+12b, EAH13].
E-C [LXD13].
Early [Kap12, Li16].
earth [Ali14, BHMN19, CZCW19, DTEMK11, SG19, ZQJC10].
easy [PR10b].
echo [HST13].
Eckart [PPK+16, TCG17, VOAH18].
Economical [ZF15].
EDA [ŠKB18].
edaravone [PGG12].
edge [PE11].
edged [WWL+11].
edges [BBK016].
edited [Ban12].
Editor [CK13, Lad14, PS14, VV13, XTIA14, C16, HS15, Luni13a, Man16, MBSAG16b, Ps13b, Sha11a, Tol13, VUC13, dSSF16a, dFR15a].
Editorial [Ano18-30, Bar16, Bri14, Cav17, For17a, Li16, LV16, MEF+15, Nag16a, Tch13].
E-... [WSML16].
ed [BAA+18].
Effect [ALRA10, BSSS19, CDldSC18, Eil14, KP10, KMM+18, KT12b, KM19, MBF11, MMC+19, Mit11b, MTS15, RP11a, Sch10b, Shi18, SYS14, WLZ+12a, YLW+13, ZCZ+12, dOLdlV13, AC19, BMTT11, BdTG11, BS14, BGL+16, Bra10, BEPZ10b, CNBPR+11, CCC19, CYLL11, COP16, DKS11,
DK13, GWZ$^{+14}b$, GZMC11, HV11, HR19, HSN$^{+11}$, IGMK11, JN13, JLG$^{+12}$, Lad14, LSR10b, LZ12, LPOP12, LWL$^{+12}$, LLC$^{+11}$, LWJL10, LB19, MNP19, MG12, MS10, MSK$^{+12}$, MPT11, MW15, NTCG18, ND10, OMK10, OA13, PCMG12, RY12, RMTG11, RRK16, RR19, SD13a, SIM14, SM19, SAHAA16, SPI14, SK10, STU19, TYN13, TM18, TJ17, WWL$^{+11}$, XTLA13, XTLA14, XWCY11, XZJ$^{+16}$, YRN$^{+11}$, YKN13, YD17, ZGSM15, ZKWZ17, dSSF16b, dSSF16a, dAVdM17, Jan10, JWG$^{+12}$, ZAE10].

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

effectively [ABM$^{+19}$. Effects [ABA11, BS16, Bla15, CAO18, KSAK17, LLZ$^{+12}$, MSRn$^{+11}$, PETB18, AGOP18, ACF$^{+11}$, Ali14, AEM$^{+12}$, ALMY18, BHMN19, BH10a, BSO16, Chr10, CFCG11, DCD11, DPDR11, DWZZ15, DOLL15, EH1K11, EKD12, EEMSS14, EAV16, Fer11, GR11, GBS17, GWM11, GZ13, GR10, GRCATG19, HZW18, Ire12, IROW10, IK14, JA12, JHSG18, KI15, KRG$^{+13}$, LDKB15, LGHL11, LDW$^{+11}$, MNZPT19, MZLM17, MKHM11, MRR13, MPE11, NG11, NMHPYG12, Oni10, OGVG18, OK19, PCR$^{+11}$, PWP13, QHS11, RLTAT19, RP11b, RFN$^{+12}$, RSL2a, RSN12, RSM12, RdA11, Ril10, SH18a, SKT115, SP19, TK16a, TV13, TFSRM11, TH12, Tob19, VFC17, VSMK13, WDR$^{+11}$, XZJ12, XZC12, XD$^{+10}$, YZW$^{+15a}$, YMY$^{+13}$, YT14, YFY17, ZHI12, ZLS$^{+18}$, ZBG$^{+19}$, ZIL$^{+13}$, ZBBB17, ZFC12, dCDC$^{+11}$, dSMT18, dSNBG08, SMK$^{+12}$].

Efficiency [Cal10, AGOP18, ATPRV11, BDG17, Mai14, THSR13, VRO$^{+12}$. Efficient [BL16, KI15, SHW$^{+13}$, SCBP17, YM14, ZWSF16, ZRLV10, CKB$^{+19}$, FH1$^{+18}$, FM16, IIS$^{+17}$, LCK$^{+16}$, OAA19, SKLC19, SGH10, SAHAA16, WTP$^{+19}$, WZX15b, ZC116, ZKW17, dSM19a].

EGEE [LG10].

Ehrenfest [KUY16].

eigenfunctions [PMGMGR12, PBR18].

eigenstates [KB12].

eigenvalue [Mit11c].

Eigenvalues [Mit11c].

eigenvector [LHX$^{+19}$. eight [SALK19].

eight-vertex [SALK19].

Einstein [DCC11].

electric [BL16, KI15, SHW$^{+13}$, SCBP17, YM14, ZWSF16, ZRLV10, CKB$^{+19}$, FH1$^{+18}$, FM16, IIS$^{+17}$, LCK$^{+16}$, OAA19, SKLC19, SGH10, SAHAA16, WTP$^{+19}$, WZX15b, ZC116, ZKW17, dSM19a].

electrochemical [AVG19b, NBZG16].

electrochemistry [FFPD16].

electrode [KK13, Sliv13].

electrodes [Che13].

electrodynamics [FNT16, IFT14, Lin14, Liu15b, Liu16].

electrolyte [DLO16].

electrolytes [AVG19a, MNE$^{+13}$, Pha19].

electromagnetic [Bae14, NTGC19].

Electron [Bas11, DZ012c, DJ18, DSVP15, LC16, LRMAA19, LZ10, MT11, PUH$^{+11}$, PI16, RVNP12, RBVAG18, SLG11, VBC$^{+12}$a, AA11, AOT$^{+18}$, Ali14, AEM$^{+12}$, AGG$^{+18}$, ALRAE11, AM18, ARH$^{+13}$, AST16, AT18, BKL$^{+13}$, BHMM19, Ber13a, BL10, BL11, BSSS19, BKM15, Bu10, Bu11a, CM13, CW13a, CM15, CG12, CH17, CSMZ10, CSTA16, DCLB15, DAA16, DLJT14, DTEMK11, Dil13, DZO12a, DLA10, Dun12, DSSM18, ETGLMJ$^{+19}$, FYHC11, Fin15, FA17, FMMD$^{+10}$,
GAPK$^{+19b}$, GS$_{A}Y_{11}$, GTR$_{11}$, GS$_{10}$, HSN$_{18}$, JdL$_{08}$, Jan$_{10}$, Joh$_{17}$, KWLS$_{15}$, Kar$_{12c}$, Kha$_{16}$, KPL$^{+17}$, Kit$_{15}$, Kri$_{13}$, KM$_{19}$, Kuz$_{19}$, Lai$_{10}$, LCH$_{14}$, LZZ$^{+11}$, LWY$_{13}$, LYL$^{+12}$, LGI$_{2}$, Lu$_{10}$, MGI$^{+11}$, MR$_{12}$, MW$_{16}$, MJ$_{16b}$, MPD$^{+10}$, MPZW$_{10}$, MGB$_{18}$, MJ$_{11}$, MNS$_{11}$, NA$_{14}$, NCMC$^{+18}$, NIK$_{19}$, NBGZ$_{16}$, NAK$^{+17}$, Nes$_{12}$, Ng$_{12}$, NDM$^{+12}$, NEI$_{11}$, NRGs$_{11}$, NMV$^{+14}$.

**electron** [OAT$^{+13}$, POLV$_{12}$, PL$_{11}$, Pir$_{13}$, PNC$_{19}$, RBGGM$_{18}$, RNV$_{12}$, RCM$_{10}$, RAGM$_{10}$, RS$_{13}$, RKCK$_{19}$, SDS$_{19}$, SDS$_{20}$, SS$_{10}$, SM$_{11}$, SBM$^{+11}$, SMB$_{16}$, SYK$^{+12}$, SPD$^{+18}$, SSAM$_{13}$, SHS$^{+13}$, SM$_{12}$, Sit$_{15}$, SL$_{13}$, ScBsr$^{+10}$, SBKJ$_{18}$, SRI$_{18}$, Tob$_{19}$, TC$_{12}$, VF$_{13a}$, VBC$^{+12b}$, WLS$^{+19}$, WWD$^{+15}$, WHI$_{12}$, XYS$_{10}$, YNL$_{18}$, YM$_{14}$, YRN$_{11}$, YHLC$_{15}$, YD$_{17}$, ZDO$_{10}$, ZFS$^{+11}$, ZZZ$^{+18}$, ZSZ$_{14}$, ZJS$_{13}$, dAI$_{12}$, dCDC$^{+11}$]. **Electron-density** [RBVAG$_{18}$]. **Electron-group** [WH$_{12}$]. **Electron-muon** [RAGM$_{10}$]. **Electron-N** [SSAM$_{13}$]. **Electron-pair** [LRMAA$_{19}$, MT$_{11}$, WH$_{12}$]. **Electron-proton** [DLCB$_{15}$]. **Electron-rich** [YNLD$_{18}$]. **Electron-withdrawing** [BSSS$_{19}$]. **Electronegativity** [CG$_{12}$, GI$_{11b}$, GI$_{11c}$, GI$_{11e}$, GI$_{11f}$, Kan$_{18}$, TSBSM$_{12}$]. **Electronic** [AB$_{16b}$, AC$_{19}$, AGB$_{19}$, AVG$_{19b}$, BZBZ$_{13}$, Ber$_{13b}$, BVP$_{14}$, BBYZ$_{18}$, BBAL$_{12}$, BG$_{11b}$, BG$_{11c}$, CZLD$_{17}$, CJGTL$_{12}$, DLLA$_{10}$, FMO$^{+11}$, FMCA$_{11}$, GZF$_{13}$, HHCA$_{10}$, IA$_{13}$, KK$_{11b}$, KLZQ$_{15}$, KP$_{13}$, LDsdMi$_{14}$, MLY$^{+16}$, MFZ$^{+18}$, MS$_{14b}$, MKM$_{11}$, NBL$^{+14}$, NDM$^{+12}$, Pup$_{11a}$, RKM$_{12}$, RZC$_{13}$, SGC$_{13}$, SBB$_{16}$, TNT$_{18}$, TSKN$_{12}$, TSH$_{17}$, VSN$^{+11}$, VBO$^{+15}$, XTLa$_{13}$, XTLa$_{14}$, YW$_{11a}$, YH$_{14a}$, AEGKZ$_{12}$, AO$_{12a}$, Alc$_{13}$, ART$_{08}$, AST$_{16}$, BVCAP$_{12}$, BPVDB$_{11}$, BPL$_{13}$, BS$_{11}$, BL$_{10}$, BW$_{15}$, BB$_{16}$, BSV$_{12}$, CWL$^{+13}$, Cas$_{15}$, CMCN$_{11}$, CWW$^{+16}$, CHSO$_{13}$, COP$_{16}$, DIOG$_{12}$, DAR$^{+11}$, DCY$_{12}$, DD$_{17}$, DWX$^{+16}$, DG$_{19}$, DCHC$_{11}$, DHYC$_{19}$, DHZS$_{11}$, DSH$^{+13}$, DB$_{13b}$, Dun$_{15}$, Dy$_{16}$, ETGLMJ$^{+19}$, Fin$_{14b}$, FSM$_{11}$, GB$_{17}$, GAPK$^{+19b}$, GSZ$_{10}$, GWM$_{11}$, GFB$_{12b}$, GP$_{13b}$, GMT$_{16}$, GEL$_{18}$, GJ$_{18}$, GB$_{13}$, GM$^{+18}$, GC$_{19}$, HMI$^{+15}$, HTM$_{10}$, HILI$_{19}$, HIJ$_{13}$, HWW$_{18}$, HhGqZz$_{17}$, IGMK$_{11}$, IK$_{18}$]. **electronic** [JL$_{12a}$, KG$_{17}$, KRF$^{+17}$, KMF$^{+11}$, KCK$_{14}$, KJ$_{15}$, KJ$_{16a}$, KJ$_{16b}$, KSD$_{10}$, Klec$_{11}$, KYLC$_{19}$, KSY$^{+11}$, KFY$^{+12}$, KZZ$_{13a}$, KHH$_{10}$, KAOB$_{11}$, KMM$_{16}$, Kri$_{13}$, KO$_{12}$, KUY$_{16}$, Lai$_{11}$, Leh$_{19c}$, LL$_{11}$, ILBqD$^{+19}$, LMZY$_{15}$, LL$_{19}$, LLZ$^{+14}$, LBdV$_{16}$, DVMC$_{19}$, LHL$^{+15}$, LZ$_{10}$, Lya$_{14}$, MSG$_{16}$, MLC$^{+11}$, MC$_{11b}$, May$_{14}$, MMW$_{11}$, MUNZVR$_{12}$, MBA$^{+13}$, MPZW$_{10}$, MGB$_{18}$, Mi$_{12}$, MS$_{17}$, MKD$_{19}$, MA$_{11a}$, MA$_{11b}$, MMRRA$_{10}$, MJ$_{11}$, MB$_{13}$, MPT$_{11}$, MPTZ$_{13}$, MM$_{13}$, MW$_{15}$, MS$_{11}$, MCR$_{16}$, MC$_{18b}$, NS$_{19}$, NA$_{12}$, NIT$_{16}$, NZAV$_{10}$, Ogv$_{18}$, PE$_{11}$, PR$_{+11}$, PAKA$_{15}$, PMA$_{12}$, QJ$_{13}$, QCB$^{+10}$, RMLPGGH$_{16}$, RS$_{12a}$, RMJ$_{11}$, RRRV$_{19}$, RNC$^{+14}$, RTMG$_{11}$, Rus$_{14}$, RMY$^{+13}$, SRPD$_{16}$, SR$_{12}$, SD$_{13a}$, SB$_{10a}$, SLC$^{+18}$, SYL$^{+18}$, SLS$^{+14}$, SX$_{12}$, SLS$^{+12}$, SLSZ$_{13}$, SIS$^{+08}$, SRS$^{+17}$, SSTO$_{11}$, SR$_{11b}$, SZZ$^{+12}$, ScBsr$^{+10}$, SSW$_{16}$, SKI$_{12b}$, TYN$_{13}$, TZ$_{11}$, TV$_{13}$, TD$_{11}$, TBB$^{+19}$, TFB$^{+11}$]. **electronic** [TRZ$^{+19}$, TG$_{13}$, UTT$_{13}$, Var$_{14}$, VPA$_{11}$, VLFG$_{12}$, WWC$_{17}$, WFS$_{13}$, WDS$_{19}$, WJL$^{+10}$, YZL$^{+10}$, YZL$^{+11}$, YZW$_{15b}$, YH$_{14b}$, ZQcJ$_{10}$, Zha$_{10}$, ZLS$_{10}$, ZZR$^{+12}$, ZCG$^{+16}$, ZQXP$_{17}$, Zho$_{18}$, ZCP$_{11}$, dSSF$_{16b}$, dSSF$_{16a}$, Bont$_{12b}$, Lad$_{14}$]. **electrons** [BEM$_{12}$, BBM$_{10}$, BB$_{10}$, BMB$_{16}$,
Dw13, Fer19, Ig11, Ign12, ISRK12, KK13, KK14a, KV19, Kry12c, Nas19, Nes10, QCB+10, RP11a, RPVM10, RS13, SALK19, She12, SS19b.

energies [BBKO16, LBW11, SCZG12, ASHF13, AC12, Ali19a, ABA11, BVCAP12, Bla15, CFCO+10, CHH’+19, DZO12c, DZO12a, EKN10, FLvLA15, FYHC11, FC19, GMA+19, GM11, GFRdG11, HNH+12, HIL19, HM10b, IKN13, Kin13, KKS+11, KB19, LDKB15, LORR+12, MIM19, Mas10, MS14c, NA14, Na13, NV10, OKR12, OK16, Pea11, PBB15, SH19, SR19, SOM10, SZL+14, TsyU15, VFS13a, VLFG12, WW17, WZ17, WR15, XCY11, YW+12c, ZZ10X, ZCC11, ZZC12].

Energy [CCl11b, FDA16, AV19, AG10b, AK17, AB18, AOLEB12, AEM+12, ART08, AZD+11, AST16, ALK19, BXR+13, BPG12B11, BP13, BAP12, BFS16, BBL12, Ber13c, BVA+14, Bou12b, Bud12, CPF+11, CWW12, CNBPR+11, CDS+18, CCL+16, CFV18, CLH14, CSG14, COP16, DK13, DB11, DHZS11, EMK14, Fin16a, FMDM+10, GST11, Gra08, Gra11, HR19, Han19, HJRO13, FHD11, HMI10b, HFdGC14, HM10b, HM11, HBMM11, ISN13, IK18, Jeo18,

F [yBZfC18, CS18, DPD11, DSSM18, DSSM19, EMSB15, GWM11, GKT+12, GB13, HNBG15, JLG+12, KAR12a, KMM16, Kuz19, LIL+11, LHGL11, LZZ+11, LMZ+11, LLG+12, LC16, MEEA+13, PP14, RLAT19, SB18, SKS10, SPI14, SYQ+10, SZL+14, TMC18, TL15, WZW17, XZL+12, MLPT10, YZW+15a, BLWJ17, DMAB12, DZO11, GKT+12, LHGL11, MA14, MGB18, Pup11b, SIK18, SZ15, TNN16, YGL+11, ZHL+19, ZCG10]. F12 [BL12, yOITn15]. Fabricio [COP16]. fac [AC19]. fac [DMWY11, DLG12]. Factor [Tri14, Kan17]. factors [AGB19, BMX+19, Mam13, MK11, SPO+11, TZ11, VLG12]. families
first-shell [JMPP19]. Fischer [MJ16a]. fischeri [PI13].
Fisher [LNV+18, MR18a, Nag15, OOI+19]. fit [Ha18]. fitting
[KFJ+18, PCV19]. five [RNV+12, WLS+19]. five-electron [WLS+19].
fixing [WR14a]. Fixation [GC18]. fixed [IM15]. flavonoid [DS18].
flavonols [FZX18]. flavor [Tch16]. flavors [Mat02, Mat10]. flexibility
[LB11, MB11, OMD13a]. flexible [BAB+18, ZP16]. flexible-cluster
[BAB+18]. FLi [YLWrL12]. flow [FUE+12]. fluctuation [NTCG18].
fluence [HMH+13]. fluid [TTM16, Vki11a]. fluids [SA18]. fluorene
[BCAP12, Shi18]. fluorescent [BBM17, LDKB15, NTCK13, TCM+
12, ZWLC12]. fluoride [HL19, LWZ+14, MtAdCS12, OCB+10, ZL10,
dLRR11]. five-electron [WLS+19].
}

...
CD12, DWJZ11, DCBB11, DKS11, DW12, DZ11a, DGR+16, DG19, DSZB18, DQZF12, ED16, FCS13a, FCS13b, FZX18, FO10, FDNR10, Fin17, FA17, FS16, GPFV19, GCK+17, GMR18, GM11, GGD12, GHCDCM1Q17, GD11, GCZ+14, HMA+19, HR19, HHCA10, HLZ+14, HZZ+19, HMH10a, HMH10b, HK11H3, HY11D, HZZ11, IN15, JR12, JPP+11, JA12, JS17, JW18, KME+18, Kar13, KPCV18, KK14b, KKL+16, KSAK17, KYLC19, KSG+12, KJ14, Kri13, Kry12c, KG08, KMU+13, Lat13, LPO+12, LSR10b, Lle19a, Lle19b, LW11, LWL+12, LWX+14, LBY+14, LLW+11, LKK+16, functional [LDZG16, LLZ+12, LSC+18, LNI12, MYZ+10, MLV+14, MJ16a, MLC+11, MFF+12, MA10, MW16, MUNZ1R12, MG12, MKG13, MLK17, MLB+12, MBBT+12, MM13, MKW11, MCRS16, MOH+12, Nag15, Nag17, NH18, NDP10, NTLN10, NL11, NMIP14, NMSR14, NDM+12, NZAV10, OD16, POLV12, PS10b, PS14, PI+13, PMH+16, PABS16, PP16, PTH11, PR10b, Pir13, PU14, PJ1P10, PMAP12, PI16, PC13, QHS11, RGPZ13, Rs12b, RCM+19, RPVM10, RAMB18, Rud12, RSCS10, SB18, SA18, SGL+16, SVRG12, SLC+18, SN12, SAHG11, SHL+13, SJZ+18, SIS+08, SDM12, SRMB15, Srl19, SK12b, SS13, TOSN12, Tan12, TIN13, Tan13, TDOD17, TFZ+15, TLC+17, UV18a, UMS13, VPGC12, Ven12, VUC13, Vik13, VBO+15, WKE17, WJL+11, WW11, WY15, WY15, WZT+11, WR15, Wit18, XNL+14, XSLF12, XGH+18b, YLH+19, YWH12a, YWH12b].


Fundamental [Brä13, Hor13, IFT13, MSH13, Mar13, YK13, ZJS13, B15, CK13, Gi11b, Gi11c, Gi11e, VVVB10, VV12, VY13]. fungal [VGS10]. furoic [VGS10]. Further [Jor15, ZLW16]. furylfulgide [LZZ+17]. furylfulgimide [LZZ+17]. fused [RGTS11, WDS19, Yaml1]. future [BJ17, MGN14, Sic16]. fuzziness [Tch16].

growing [CD12]. growth [LVP12b]. Grx3 [Dum12]. Grx3-like [Dum12]. 
GTP [MMT+13]. guanidine [LW13]. guanidine-catalyzed [LW13].
Guanine [SL10, BSV12, KMMS17, POLV12, YM12, ZRY+13]. guess 
[LCK+16]. Guest [DC14a, XXbX+13]. guests [NCMC+18]. guide [SLS+19].
guided [SRS+17]. Guseinov [Mam14]. Gutzwiller [YWH12a, YWH12b].
GW [RAMB18].

H [BDF+18, BGFD14, BJ17, BTH18, Buc12a, BSPK11, CRSB12, CS17,
DMAB12, DPDR11, DZO11, DZO12b, DQZF12, EML+11, EMS16,
FBRBR12, GWMI1, GB13, GR10, GKG18, HJRO13, JCCZ12, JLG+12,
KWC10, Kal18, Kun11, Ki12, KSSK16, KSST12, KRG+13, LZ12, LCL+10a,
LJ+11, LZZ+11, LMZ+11, LBY+14, LZW+15, LCZ15, LXD13, LdAA+11,
LEU+11, MLY+16, MC12, MMBK12, MPRB+10, MC18a, NBL12, NL11,
NMPI14, NH11, OCL+18, PTS+11, Pan16, QSLY10, RLTAT19.
RFEGPP+16, RGR12, SBAT16, Sat11b, SZZZ11, SCTW10, SZL+14, SZ15,
SY17, TBRIS12, TG13, Vlk+11, WCY+10, WZW17, WLL14,
WWGW18, XLLZ10, XCL+18, XF19, Y1Y+13, YSK+12, YLYC18, ZGSM15,
ZCG+17, ZWL18, ZHL+19, AC12, AST19, BN12, BDFM10, BPVDB11,
P13, BPG+10, BAP12, BEM11, BHV+11, Buc12a, CLXZ12, CP10, CC11b,
Cor16, DLCB15, DSA18, Den13, DMS+10, DLM12].

H-Bond [LCM+11, SMEH16]. H-bonded [DLM12, DMBL16, IS08, IKS10].
H-bonding [CLXZ12, DMS+10, KdPNN16]. H-bonds [IROW10, SS11].
H-passivated [GMT16]. H/D [SK10]. H2 [ZCG+17]. H5N1 
[KRH13, WZ10a]. HAI [Sat11a]. HALA [RKR16]. Half 
[KMS+11, AAAM12, AAA12, DZO12b, SMOD11, Pup11b]. Half-a-century 
[Pup11b]. half-line [SMOD11]. half-metallicity [AAAM12, AAA12].
half-sandwich [DZO12b]. halide [DZO12c, HNBG15, LGM+18, XZL+12].
halide-exchange [XZL+12]. halides 
[BMBD10, For12, LC16, MML+11a, RYM12, RKCK19]. Hall [Bra10]. halo 
[EMK14, LGP+11]. halo- [EMK14]. haloalkane [ZCZ+12].
haloammonium [XZL+12]. Halogen [DLP17, SC18, VVY18, BLL+13,
Buc11b, CLXZ12, DPK18, DWZZ15, EMSB15, FGD+19, GLXL18, JZL+17,
KCC14, Kuz19, LLJ+11, LLG+12, LDG16, LDZ+11, LLZ+12, MS14c, Sch13,
SMP10, SPI14, SY16, SCZH16, TL15, VVJ15, WTW+15, XZYS10, YZZ16,

hexafluorocyclohexane [HWWW18]. hexagonal
[KC19a, LFP+19, NBL+14, PL18a, UV18a, UV18b]. hexahydro [MJ11].

hexahydro-1 [MJ11]. hexanal [BCS+12]. hexanuclear [PAPCM+16].
HF [GKT+12, LGW11, SPI+14, YGL+11, YZ10, AFM+10, SY+16, SCZH16, Boul2a]. HFC [Tas14]. HFC-32 [Tas14]. HFE [KAR12a]. HFE-161 [KAR12a]. HFF [BLKB11]. Hg [NF+11, WHM14]. HgClO4 [RSM12].

HGGGW [MRT11]. HH [Che12]. HI [LGW11]. hidden [YLZ+17].

Hierarchy [ZLE17, PC13]. HIF [MK+12]. HIF-1 [MK+12]. High
[Beh15, LGW11, Beh15, BHH+13, CKB+19, CRFR11, CL14, CKYR18, CML+16, DBTA19, DSFT17, DSSM18, Fer11, HSN18, Jeo18, JW19, KG17, KMU+13, LCL+10a, cLqFtW14, LMC19, Luz08, Lya19, Mai14, MDC15, Mili2, NKKN15, RTGS11, RNE10, SSP+17b, SZL+14, WCGD12, fXXBhD19, XZZ+10, XCD18, YYY+12, YZ13, YMI4].

high- [Fer11]. high-density [JW19]. high-dimensional [Beh15, DBTA19].

high-efficiency [Mai14]. high-energy [CL14, XZZ+10].

high-energy-density [Jeo18, fXXBhD19]. high-harmonic [CML+16].

high-level [LCL+10a, RNE10, SZL+14]. High-lying [ZCG10, DSSM18].

high-order [Luz08]. high-performance
[BBH+13, CKB+19, cLqFtW14, Lya19, NKKN15]. High-precision [Kin13].

high-pressure [KMU+13]. high-resolution [DSFT17].

High-spin [MPRB+10]. High-temperature [Dun15, WCGD12].

high-throughput [CRFR11, KG17]. high-valent [YYY+12]. higher [LBW11, SMRK18].

highest [SM14b]. Highly [KPH+12, KS18, WZW17, EM19, KRH13, LLZaH14, NDH10, OK16, OAA19, SMEH16, YAF+15]. hill [SSB12a, RA10a].

Hillman [QZW+17]. hindered [SBEH11]. Hirsch [MC18a]. Hirschfelder
[Haj18]. Hirschfelder-long-range [Haj18]. histidine [NGH+12]. histone
[dSMPRP18]. Historical [Hop15]. hitting [PR11a]. HIV

HMgH [WLL11]. HMgO [LGP+12]. HMH [BLB+13].

HMX [Jeo18, LZZ+13]. HMX/NOTO [LZZ+13]. HNB [LCL+11]. HNBe
[LCL+10b]. HNCh [XDM+10]. HNgBeF [SMC18]. HNO [BL11, YL10].

HOAI [LGP+11]. HOCl [RNE10]. Hoff [Buc10]. HOH [SW12].

Hohenberg [LB14b, Lev10]. holding [NIK19]. hole
[ATPRV11, ABLT11, FY11, JLG+12, MCL11, SC18, VATPR11, VAT12, WTP+19, WLC+17, ZHL+19]. hole-transporting [MCL11]. holes [CP13].

hollow [MC18a, PAKA15]. hollow-caged [PAKA15]. Holstein [DTFK15].

HOMg [LGP+12]. HOMO [MA12]. homodesmotic [MMM19].

Homodimers [ZS12]. homogeneous
[CSTA16, Lak10, MLB+12, MMM+12, Sic16, Yak10]. Homology
[PTD+12, SLS+10, CSVCB12]. homolytic [KZA+17, OKR12, OK16].
59
Homonuclear [EMS16, KBGC12, NZ13, SZZ+ 19, SM14a]. HONPAS
hopping [MMG15]. horseradish [ZST+ 10]. HOSO [STU19]. host
[DC14a, MSS11, OCGM+ 19, XXbX+ 13, YBMK12]. hot [BW15]. HOX
[LLG+ 12]. Hras [MMT+ 13]. Hras-GDP [MMT+ 13]. Hras-GTP
[MMT+ 13]. HRh [DPDR11]. HS [dDGNB10, LZFZ13]. HSAB [ZXY13].
HSAl [LPG+ 12]. HSH [SKS10]. Hsp90 [KTI+ 12]. HT
[CSVCB12, CSSK+ 12]. Hua
[FKBG19, HYZS19, KBG17, AAHN16, HRT12, HYZS12]. hubbard
[LNI12, HFdGC14, WDJ+ 17]. Hubbard-corrected [HFdGC14].
hubbard-like [LNI12]. Hückel [Koc13b]. Huge [FBD+ 13]. Hulburt
[Haj18]. Hulthén [Roy15]. Human [CSVCB12, WTH+ 11]. humans
[KRH13]. Hund [KT12a, MHT+ 08]. HX
[SPIL14, HNBG15, SPIL14, Vie17, Wu11]. hybrid
[AV19, AF16, Ali19a, AK11, CF14, FCS13a, FCS13b, HZZW11, Kry12c,
KSO19, LPO+ 12, MCK17, NMSR14, SB10b, SX15, TFSRM11, XCY15,
YYI+ 12, YIY+ 13, Yu13, YF16, ZPR10, MPE15, SIS+ 08, YSK+ 12].
Hybrid-density [SIS+ 08]. hybridization [ABS11]. hybrids [MJM19].
hydantoin [ND11]. hydratase [MLW+ 14]. hydratase-lyase [MLW+ 14].
hydrate [XXbX+ 13]. hydrated
[BMF+ 14, EPS+ 16, MNC12, SMEH16, SCS15]. hydrates [LB19].
Hydration [Ma14, Pat15, PBM10, RGR12, RBTL19, SL10]. hydrazide
[DDÇY12]. hydrazine [SC12a]. hydrazono [KDÇ12, SC12b]. hydride
[BLL+ 13, Ber13a, HMI+ 15, JL12b, Mar11, MHOG18, OA12, YYS15].
hydrides [AO12a, BDR12, CP13, EAA17, SH18a, SSA18]. hydroacylation
[WML10]. hydroaminations [ZSS+ 13]. hydroboration [SLS+ 15].
hydrocarbon [MSY+ 12, WLS+ 19]. hydrocarbons [BRS10, Bla15, CA17,
DI18, FC19, GMT18, GHS12, HIL19, LVP12b, RNV+ 12, SFM13, VRO+ 12].
hydrochloric [dLdOdAD12]. hydrofluoropolyethers [Vie17]. Hydrogen
[AO12a, BLR12, BAP13, Cha10, CTDOLA10, GZ14, HS15, JLG+ 12, KK11a,
MSVMCI10, MURR13, ND11, NBL12, OA12, PCMG12, SGKG12, SJZ+ 18,
SKM11, WWGW18, YL10, dFR15a, dLRR11, AV19, AKHS13, BCGC12,
BN12, Bay19, BL11, BWB+ 18, CdLdSC18, CDS+ 18, CNSK11, CCP18,
CC11a, Coo12, COP16, DAC11, DAC12, Den13, DLG12, DLM12, DLP17,
DB15, EKN10, EPS+ 16, FAFR12, FRNM12, FMCA11, FKC12, GI14, GIO12,
GH11, GORW19, GZBH18, GZMC11, HNH+ 12, HL19, HNBG15, HYD11,
IAA15, IK18, JN13, JCCZ12, JZZH17, Kar12c, KKG12, KS18, Kry10,
LLF+ 12, LJW+ 11, LLG+ 12, LWX+ 14, MS14a, MdAdCS12, MK11, MK12,
MNV+ 17, MCARL11, MTL+ 12, MT10, MFOH18, MFLK11, MMBK12,
MS14c, MMM+ 12, MAPS18, MNS11, MR18b, NW12, NG11, NMIP14, NH11,
NHB12, NRGS11, NRP+ 11, NRHJ11, NEEV15, OH12]. hydrogen
[OH13, OHDA13, OA13, PM17, Pup11a, RZ17, RZSZ18, RJY+ 10, RJA+ 10,
RYM12, RI19, Ril10, Riv11, RAFR18a, RAFR18b, RNE10, RB11b, SRPD16,
SS10, SMRK18, Sch10b, Sch13, SK17a, SM19, SMP10, Sic16, SSP14, SPIL14,


hydrogen-bond [OHDA13, SCL19]. Hydrogen-bonded
[SGKG12, CdLdSC18, CCP18, KS18, LJW+11, MT10, OA13, RNE10, ZLZ+14, dSCC12]. hydrogen [OHDA13, SCL19].
Hydrogen-bonded [SGKG12, CdLdSC18, CCP18, KS18, LJW+11, MT10, OA13, RNE10, ZLZ+14, dSCC12]. hydrogen-like [SS12].
Hydrogenated [IIW+11]. hydrogenation [TGA+11, VPGC12, XSLF12, ZZC15].
Hyrogenic [DLRMFY10, DBTA19]. hydrolysis [CCL+11, DSZB18, KFS13, PRFR17, PMC11, RNDA+10, YTY19].
Hydronium [DE18]. hydrophobic [NHG+12, SMK+12]. hydroquinone [NP18].
hydrosulfide [HLJZ11]. hydroxamates [TPdMB12]. hydroxamic [KK11a].
hydroxide [DE18, RGR12, WZZL10]. hydroxides [DCDD10].
hydroxy [TAY11, YLW+13]. hydroxyacetone [SSdS17].
hydroxynaphthoquinone [JB11]. hydroxybenzaldehydes [EKN10].
hydroxybenzenes [ATM17, KM12a]. hydroxybenzylamine [AF+10].
hydroxycarbene [Buc12b]. hydroxycarboxyls [SSdS17].
hydroxycinnamoyl [MLW+14]. hydroxycinnamoyl-CoA [MLW+14].
hydroxyl-fullerene [KK11c]. Hydroxyl [TWHZ14, CGIAI12, FNBK17, KAR12a, LLP+13, LCM+11, Ril10, XNL+14, YMY18a, ZZC12].
hydroxyl-thiourea [LCM+11]. hydroxylapatite [UV18a, UV18b].
hydroxylated [MDND+16]. hydroxylations [SSI+10].
hydroxylbutyloxy [RS11b]. hydroxylbutyryl [MFR10].
hydroxynataresinol [SBEH11]. hydroxymethyl [KAOB11].
hydroxyphenalenone [OA13]. hydroxypropanal [SSdS17].
hydroxyquinoline [CHV14]. Hylleraas [OH19, PSGK17]. Hyper [LXW+12, DW12, FK1+12, KP11, Kha16, Mar12, XWCY11].
hyper-netted-chain [DW12]. hyper-radial [Kha16]. hyperbolic [AY15, GE12b, SDL+15, dAB17]. hyperbolic-type [AY15]. hyperbolic [WC14].
hyperconjugative [CSP+10]. hyperfine [Bou11, Bou12a, Kin13, Wit18]. hypergeometric [PMGMR12].
hyperpolarizabilities [AK11, CEFMK12, NKF+13, OCL+18, YMY+13, dWLC14].
hyperpolarizability [BHMN19, FSB16, GXZ+14, Kar12b, Mar11, RVO+14, WWL+11].
hyperspherical [BAP12, PML+11, RPB11]. hypersurfaces [PBM10].
hypervirial [ATPRV11, VATPR11, VAT12]. hypochlorous [TV13].
hypoelastic [SALK19].
identical [XLz+12]. identifies [ST15]. identify [MVG18].
Identifying [BB16]. identities [Cin11a, Cin11b].
Identity [RDB19, Buc10, Buc11a, GI11b, GI11c].
IEO [FYhC11], IEPOX [KZZ13b].
II [Bal16, DSD18, DCdG10, FBD+13, LYW11, LGW11, LGS+16, MGK19, NNSN17, NFQ+11, OAA19, RNdA+10, SLC+18, SG19, TFA10, WHM14, WRW+18, YZL+10, ZSASS13, ZLLS10, dCSDdMC13, dARAV12, dCDC+11, ADR+18, Bou11, Bou12a, Cam10, CPF12, Ire12, Jor18, Kry12b, Leh19b, LSR+13, MS12, OH13, PDI1, PEA+12, PVS12, QD10, SGL19, YVI+13, YIY+13, YSK+12, YWR+18]. IIB [Eng16].
III [CADSG18, EG10, LD5dSI14, MSOV13, MMSC19, PCD14, RMP+14, SLS+14, SSP+17b, SHW+13, WXH+11, ZQCI10, ZQJR13, ZSYW17, ZSQ+10, AC19, AMK10, Cam12, CWS15, LCR+17, NMS+10]. IIIA [Eng16].
Illustrative [Mai14]. Image [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h, Ano13a, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13k, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13x, Ano13y, Ano13z]. Image [Ano14a, Ano14b, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z]. Image [Ano14a, Ano14b, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z]. Image [Ano14a, Ano14b, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w].
Ano19], Ano19k, Ano19l, Ano19m, Ano19n, Ano19p, Ano19q, Ano19r, Ano19s].
imidazo [YZW+15a, YB11]. *imidazole* [CC11a, NHG+12, ÖEDB11, VHTEG15]. *imidazoles* [Tug13]. *amine* [BH10a, ÇT14, Coo12, HS11b, LFTL18]. *amines* [SFW12, XZG+18, ZZC15, ZQW+17]. *imino* [BSM+15, HNH+12, ¨OEDB11, VHTEG15]. *imidazoles* [Tug13]. *imine* [BH10a, C¸T14, Coo12, HS11b, LFTL18]. *amines* [SFW12, XZG+18, ZZC15, ZQW+17]. *imino* [BSM+15, HNH+12, ¨OEDB11, VHTEG15]. *imidazoles* [Tug13]. *imine* [BH10a, C¸T14, Coo12, HS11b, LFTL18]. *amines* [SFW12, XZG+18, ZZC15, ZQW+17]. *imino* [BSM+15, HNH+12, ¨OEDB11, VHTEG15]. *imidazoles* [Tug13]. *imine* [BH10a, C¸T14, Coo12, HS11b, LFTL18]. *amines* [SFW12, XZG+18, ZZC15, ZQW+17]. *imino* [BSM+15, HNH+12, ¨OEDB11, VHTEG15]. *imidazoles* [Tug13]. *imine* [BH10a, C¸T14, Coo12, HS11b, LFTL18]. *amines* [SFW12, XZG+18, ZZC15, ZQW+17]. *imino* [BSM+15, HNH+12, ¨OEDB11, VHTEG15]. *imidazoles* [Tug13]. *imine* [BH10a, C¸T14, Coo12, HS11b, LFTL18]. *amines* [SFW12, XZG+18, ZZC15, ZQW+17]. *imino* [BSM+15, HNH+12, ¨OEDB11, VHTEG15]. *imidazoles* [Tug13].
[SKY^{13}, DLLA^{10}, FBD^{13}, OG^{19}, YTY^{19}]. influencing [BMX^{19}].
inhibition [AI^{11}, PCF^{18}, THSR^{13}]. inhibitive [LZB^{10}]. inhibitor [SKHN^{13}, SKS^{10}]. inhibitors [DSWL^{11}, EAK^{10b}, EAK^{10a}, KMRG^{13}, KKG^{12}, MGK^{12}, RDM^{11}, ST^{15}, SLA^{12}, TP^{14}, WLL^{13}, YFW^{14}, YWY^{12}, ZFW^{13}, dOdONM^{12}]. InI [BD^{12}]. Initial [BLWJ^{17}, BS^{16}, LCK^{16}, Liu^{15a}, TJS^{17}]. initialization [ZWSF^{16}].
TSL11, THVP14, UGWL18, UV18b, VPFD10, Var11, WZX11, Wit18].

initio [Wu11, WIWL14, YKM+15, YZL+11, Yu13, ZDZO10, ZZL+11, ZLZ+14, ZF15, ZXY13, ZZZ+18, ZRL10, DAE+12, GWJ12, MPM15, SW12, Wag14].

initio-based [LV12].
injection [ZQJW13].
inner [BB10].
inner-transition [BB10].
intrusion [LV12].
injection [ZQJW13].
inner [BB10].
inorganic [BMRM19, BMF+14, BGJSM+18, KSO19, MCCGM+19, Swa13, YSA+11].
inserted [KRH13, Lwl19].
insertion [DPDR11, RRVJ10, SMC18].
Insight [DMWY11, HFL+17, She12, She13, TFZ+15, WLL+13, BGMD15, GR+16, EM17, KCDC15, MNV+17, MC17, MMSC19, RNd+10, SAG13, SACA18, SC11, VIHTG15, YWJ+11, AF16, Tan13].
Insights [CP13, CADSG18, GJ18, HNBS18, MS14a, MC18b, SLA12, TFBG14, VBO+15, Bal16, BHA19, DJB10, LXW+14, LKZ+16, MNE+13, NP18, Pan16, SMGZF19, SR11a, SKB18, XZYS10, XLZ+19, YHLC15, dSM19a, dARAV12, KMS+11, QTCL10].

Instability [Pat15].
instanton [Buc12a].
insulator [BEM11, Lar12, SAHG11].
superscription [BMRM19, BMF+14, BGJSM+18, KSO19, MCCGM+19, Swa13, YSA+11].
inserted [KRH13, Lwl19].
insertion [DPDR11, RRVJ10, SMC18].
Insight [DMWY11, HFL+17, She12, She13, TFZ+15, WLL+13, BGMD15, GR+16, EM17, KCDC15, MNV+17, MC17, MMSC19, RNd+10, SAG13, SACA18, SC11, VIHTG15, YWJ+11, AF16, Tan13].
Insights [CP13, CADSG18, GJ18, HNBS18, MS14a, MC18b, SLA12, TFBG14, VBO+15, Bal16, BHA19, DJB10, LXW+14, LKZ+16, MNE+13, NP18, Pan16, SMGZF19, SR11a, SKB18, XZYS10, XLZ+19, YHLC15, dSM19a, dARAV12, KMS+11, QTCL10].

Intelligence [Ezz10, SRS+17].
Intense [DLCB15, SRP+16].
Intensities [VVVB10].

Inter [BR16, COP16, HS15, Man16, dFR15a].
integral [HSN18, HFB11, KSST12, LWY+13, Mak15, RGLV+14, SGC13, YK13, ZLR15].
integrals [AE¨O12, AA15, GTR11, GS10, Hog10, YM14, YSÖ12].
Integrated [Cap16, HCH+18].
integration [BG11a].
integrations [Koc13a].

Interaction [ASHF13, DWPK14, EG10, JLS13, MYZ+10, MRT11, RNB+10, SPD+18, SK11, TBRIS10, ZT13, Ali19b, Bae14, BLL+13, Bas11, BEM11, Ber13b, CAZ+11, CCL+13, CGM12, CGG18, CRSB12, Cha10, CC11a, CYL+18, CP16, DC14a, DVBDM11, DTVP+12, DLG12, DWZZ15, ELC08, Eng16, EBH11, EAV16, FZX18, GWZ+14b, GD11, HFD11, HM10b, JFT13, JH15, JLG+12, KMM+18, KV19, KPH+12, LLG+12, LBdV16, LuO8, MMR+10, Mar12, MMC+19, NL11, NV10, NFQ+11, OA12, PSK+16, PR18, RYM12, RFN+12, RFMC19, RS11b, RRCO11, SB19, SA18, SD13a, SD16b, SKHN13, SYL+18, Shal1b, SLZ+11c, SS11, SM14d, SWS12, SZL+14, SYY16, SCZH16, TK16b, TG16, VIHTG15, VVVB10, WLL11, WZ17, WWQG17, W18, Wm10, Xbx+13, ZST+10, ZCZ+12, ZS12, ZMB+17, TBRIS11, TBRIS12, YL10].

Interactions [KMMS17, MKF+12, dCDC11, AGRI+12, BMIR+13, BAP12, BMRM19, BLW17, BDG17, BLDV19, BWE16, Buc12b, CNBPR+11, CdLdSC18, CNSK11, CCS13, CKL16, Chu12, CSP+10, Cys11, DJB10, Dob14, DLPL17, EAA17, EA12, EMS16, FNK17, FRGC10, FKCI12, HCH+18, HMA+19, HYD11, Ja10, JEA13, JLZ+17, KDPPNS16, KMK+16, KP12, KKG12, Kry12a, Kuv10, Kuz19, LMZ+11, LC16, LWY+19, LZZ+13, LDZG16, LB18, MBZ+13, MHZ18, MS12, MIKH19, MSNP18, MPD+10, MPPW10, MS10, MSY+12, MZLM17, MAW+18, MRR13, MMSC19, NH18, Nal13, NRI15, OA13, PML+11, PABSK16, PP16, Pie12, PETB18, RK14, Ril10, Riv11, RGR12, SB18, Sch15, SSAM13, SM14b, SM14c, SS13,
TH12, TDOD17, TCS10, Var11, VBC+12b, VSMK15, Yak11, YJ17, Yu13, YF16, YFY17, Zak13, ZRY+13, ZFS+11, ZLWZ16, dCSDdMC13.

kinetically \([\text{FXxBhD19}].\) kinetics
\([\text{ACMRN10, BMB12, BLM+12, CdAFS+12, COdF+11, DS12, EML+11, HWHZ11, MXC18, MCC12, MPREGC12, MML+11a, MLB+12, MMM+12, PRFR17, RLV+13, Var14, WLL+14, ZZW11}].\) kinks
\([\text{Yak10}].\) Kirchhoff
\([\text{Cin11a, LSW19, LWY19, PR10a, Pal10, PR11b, PR11a, PL18a, WZ10b}].\) Kitaev \([\text{TSS+15}.\) KOH \([\text{VLK+11}].\) KOH/DMSO/CH \([\text{VLK+11}].\) Kohn
\([\text{AT18, BW18, Bar11, GdSM+10, KFJ+18, LB14b, Lev10}].\) kojic
\([\text{KS11}].\) Kondo
\([\text{BRBRS11}.\) Kondo-like
\([\text{Cin11a, LSW19, LWY19, PR10a, Pal10, PR11b, PL18a, WZ10b}].\) Kondo
\([\text{BRBRS11}.\) Kondo
\([\text{Kim18, RTG+19}.\) layer
\([\text{Kim18}.\) layer-structured
\([\text{Kim18}.\) layers
\([\text{KHL10}.\) LCAO
\([\text{Dal13}.\) LDA
\([\text{Fuk12}.\) Lead
\([\text{VDG13, CAA19, MW15, Per10b, VVY18}.\) Leading
\([\text{LG12, KMS+11, YY18a}.\) Leading-order
\([\text{LG12}.\) learned
\([\text{LSP+16}.\) learning
\([\text{BR15, CKD15, FLvLA15, MJSC18, NDLC19, Rup15a, Rup15b, SKLC19, STM17, vLRRK15}.\) Lee
\([\text{LJ16}.\) Legendre
\([\text{Win10}.\) Leibler
\([\text{LSS19, LNV+18}.\) length
\([\text{Mar11, PE11, RKCK19, Sch10b}.\) Leonard
\([\text{CAPL12}.\) lesion
\([\text{SM13}.\) lessons
\([\text{PR10b}.\) Letter
\([\text{HS15, PS14, Sha11a, dFR15a}.\) Letters
\([\text{CK13, COP16, Lad14, Lun13a, Man16, MBSAG16b, PS13b, Tou13, VV13, VUC13, XLTA14, dSSF16a}.\) level
[FUE+12]. Ln [BSPK11]. LnO [TG13]. Load [NMSR14]. loaded [LWX+14]. Lobatto [Rom10]. Local [AKR12, FSST16, IN15, RB18, ZXY13, ATL+14, AK11, CCL+16, DNCKS+12, Fin17, FKC12, Glu13, ISN13, KK12a, Lya14, MDND0+16, OS10b, OPAVM18, PK13b, PSR11, RPBB11, RPVM10, SMGZ19, SN15, SACA18, Zha17, Kut13, YSS+10]. Locality [RCP14, LNV+18]. Localization [GB10, AOT+18, AT18, BEM12, BL10, BL11, GNM+12, KC18, MGB18, MFLP12, OAT+13]. Localized [ABS13, NB19, AEKZ12, ALK18, BMB10, IK18, PABS16, SS19, DG19].

Lobatto [Rom10]. Local [AKR12, FSST16, IN15, RB18, ZXY13, ATL+14, AK11, CCL+16, DNCKS+12, Fin17, FKC12, Glu13, ISN13, KK12a, Lya14, MDND0+16, OS10b, OPAVM18, PK13b, PSR11, RPBB11, RPVM10, SMGZ19, SN15, SACA18, Zha17, Kut13, YSS+10]. Locality [RCP14, LNV+18]. Localization [GB10, AOT+18, AT18, BEM12, BL10, BL11, GNM+12, KC18, MGB18, MFLP12, OAT+13]. Localized [ABS13, NB19, AEKZ12, ALK18, BMB10, IK18, PABS16, SS19, DG19].

Lobatto [Rom10]. Local [AKR12, FSST16, IN15, RB18, ZXY13, ATL+14, AK11, CCL+16, DNCKS+12, Fin17, FKC12, Glu13, ISN13, KK12a, Lya14, MDND0+16, OS10b, OPAVM18, PK13b, PSR11, RPBB11, RPVM10, SMGZ19, SN15, SACA18, Zha17, Kut13, YSS+10]. Locality [RCP14, LNV+18]. Localization [GB10, AOT+18, AT18, BEM12, BL10, BL11, GNM+12, KC18, MGB18, MFLP12, OAT+13]. Localized [ABS13, NB19, AEKZ12, ALK18, BMB10, IK18, PABS16, SS19, DG19].
NDLC19, Rup15a, vLRRK15. machine-learned [LSP+16].
machine-learning-augmented [CLKD15]. macro [RAK10].
macro-dimensions [RAK10]. macrocycle [CJMC19]. macrocycles
[VSMMK15]. macromolecules [Chr+10, OVT+16]. macroscopic
[DLML2, DP11, FUE+12]. made [Mas10]. Magic
[TB15, MJ16a, MHHPR+17, TZD+19]. Magnesium [FMP+17, BPT12].
Magnetic [GKS10, KV19, KMG+13, MPD+10, MPZWD10, WSC11, Zag11,
AGCV15, ATL+14, AC11, AK11, ALB18, AM10, BXR+13, Boli2b, CL11,
CWW+16, CKL16, GE12a, GV11, JL12a, JHL+18, KSC15, KSM+12,
KSY+11, K12h, LAc14, LB14b, LL19, LMC19, LB19, Mag14, MB+13,
MC18a, NBL+14, OMD13a, PL11, RP11a, RZC13, SRPD16, SSI+10, Shi18,
SSI2b, SSB16, SS12, Sto18, SS13, TD11, TW10, Vik11a, Vik11b, Vik13,
VRO+12, YZW15b, ZPM10, ZP16, ZLS+18, ZLWZ16, ZST+10].
magnetic-field [PL11]. magnetic-resonance [AK11].
magnetically [ATM17, ALB18, MAT19]. magnetism [ABP13, KLZQ15, SC10b].
magnetization [KLZQ15]. magneto [KG17]. magneto-electronic [KG17].
magnetolectric [RC11]. magnetoexcitons [MLDP10].
magneto-resistance [ZX12]. magnetotropicty [TG13]. magnets [LL19].
magnitude [LZD+11]. main [TMC+13]. main-group [TMC+13]. Major
[ALK19]. Makarov [Cyl+18]. make [SLS+19]. MALDI [HMH+13].
malomaldehyde [NRHJ11, RJR+10]. malonate [DdG+11, JSH].
maltolat [DdG+11]. manganese [SSK+12]. manifest [GI11e]. manifold
[TFZ+15]. Mannich-type [TFZ+15]. Manning [ZFH]. Many
[B10, GR11, CSMZ10, DLP17, Fer19, Fr12, Kha16, KRG+13, LV12, Lin14,
Lya14, Nas19, Per1a, RBVAG18, SK17b, SIB+13, SHKS15, Sit15, Zak16].
Many-body [BOS16, GR11, DLP17, Fri12, LV12, Lin14, Lya14, Per10a,
SK17b, SIB+13, SHKS15, Zak16]. many-electron
[CSMZ10, Kha16, RBVAG18, Sit15]. many-electrons [Fer19, Nas19]. map
[DW12, Dw13]. mapped [Sta10]. mapping [Kry12b, WWC17]. maps
[GB18]. Maria [HS15, dFR15a]. marker [BCNR18]. Markov [Cal10].
Markovian [CW13b]. Markovnikov [DMWY11]. Martin [TM19]. mass
[ABKJ18, Dw13, DdG+11, FUE+12, PGGRMP10, SBB18]. masses
[GbZAI0]. Massively [OIT15, PCV19]. match [SMK+12]. matching
[MGN14]. material
[FPF16, IKC18, LC12, Oun12, OA13, TFCB14, YBMK12]. Materials
[Nem14, BCGC12, BHH+13, BCNR18, CLH14, DMBL16, Fer11, GNM+12,
HNGB15, IIS+17, Jia15, KJ15, Kim18, LPO+12, MW16, MML11b, MSOV13,
MGP16, NBI+10, PETB18, SBB12a, TK16b, UMS13, VVY18, Wagy14,
fXphD19, ZCY+16, ZWSF16, ZLWZ16]. Mathematical
[Gar08, Lev16, Sha11a]. matrices
[ABL17, Boc17, Gin10, Mit11c, Per18, WH12, Yur13, Yur15]. Matrix
[LZL08, AAHN16, AOI12b, CW13a, CM15, EM16, GBK18, HMH+13, KK13,
KJ16a, KJ16b, Kit14, Kit15, KIT17, KFS13, KFJ+18, Lan10, Lat13, SHS+13,
Matrix-covariant [Luz08]. matter [AF19b, DW12, Ng12, Tap15]. Matthews [BSS16]. Matthews= [MSBF18].

Matthews= Olson [MSBF18]. Mattsson [MA10]. MAu [FTB11].


MD [AHCh+18, Eil14, MFB11, SLA12, YWY+12]. MD/QC [Eil14].

MD/QC-simulated [Eil14]. MD/QM [MFB11].

Me [ˇCFˇC11, GWM11, HHL14, RBTL19, HHL12a]. mean [DCD11].


means [AGNS14, BL10, N´em14, OK16, RNdA+10, TH12, ZXY13].

measurement [Ezz10]. measurements [Bra19, KDA+11, ZPM10]. measures [Ale13, DTPC17, IOO18, Kan18, LS17, LSS19, Lat13, LRMAA19, Luz13, MR18b, SLG11, YOS15, ZYL+14].

MeB [ˇCFˇC11]. mechanical [CPAT11, DKR10, DC14b, LV19, MMP+18b, MD/QC-simulated [Eil14].

mechanics [BBB+12b, EAH13, IAK13, Ma14, MPE15, MSC10, Rup15a, Rup15b, SK17b, SB+13, UV18b, Brãl12]. mechanics/molecular [Ma14].

Mechanism [KBF+13, MCC13b, Pli18, SH18b, WML10, ZQW+17, ZL10, AG10a, Bal16, BCP10, BL11, BLWJ17, yBZc18, CCL+10, CWS15, DS12, DP12, DZ11a, DSZB18, EAH13, EM17, FZX18, FDMR11, HWH11, HhGqZZ17, JSLH14, LGM+18, LJK+18, LLLL16, LZW+18, ILBqD+19, LS19, LWJL10, LWC+10, LCM+11, LCS+11a, LCH+11, LCS+11b, LXLL11, LLLL13, MLW+14, MOS10, MR11, MML+11a, MKW11, NE11, OH12, OH13, PL18b, PO15, PY12, RFMC19, SAS+12, SSI+10, SAG13, SLS+15, SSdS17, TM13, TY110, TXL10, VPQC12, VLK+11, VOK+18, WGLX10, WXZ+11, WHS+13, WWL17, WWX+11, WLD+10, XDM+10, XZCH11, YM12, YNLD18, YWJ+11, YZZH15, ZRGE+19, Zha10, ZZW11, ZCZ+12, ZBK15, ZBG+19, ZSL+13, ZCTG18, ZTC11, ZLY+14, ZPW16].

Mechanisms [CGIA12, LLFI17, LFTL18, PWL+10, XZG+18, AGNS14, CWZ+10, FTB11, HLS11, HHZ+19, HB18, HY13, JLS13, LNGW14, LD17, MXC18, MMP+18b, MLB+12, NKWT19, NZLG15, OD12, PTS+11, PRG+10, RFEGP+16, SYK+12, SSK+12, SS18a, VHTEG15, WLWT12, YSS+10, ZPB12, ZM13, ZSHL16].

Mechanistic [Buc12b, GMT18, LTL18, LKZ+16, NP18, SGL19, WRW+18, dSM19a, AASU+17, AEAS+19, RNdA+10, VPQR19, dLIAI+12]. mechananochemical [TJS17].

mechananochemistry [QBR18]. media [CFL15, Ser11a].

mediated [Dau16, FDMR11, SGL19, WTP+19, ZL10]. mediating [Var14, ZYL+14].

Medium [TBRI12, BRS10, BB16, EAK+10b, EAK+10a, MP1+11, PBB15, Puz16, Ser11b, TV13, TBRI10, TBRI11, XDM+10]. medium-sized [Puz16]. medium-to-large [BBB16, PBB15].

MEDT [ZRGE+19]. meeting [Tch13]. Meetings [AIKVZ12]. meets [Puz17].

melamine [AASU+17]. member [RNV+12].

member [ABTW14, BBKO16, MSK11, VsRSW+11, Zha14]. membrane [FPM+17, KMT+12, SMK+12, YINM13, MPM11]. memory [BXR+13].
MMA10, MB12, NZ13, NL11, Ols11a, Pu11, SBMM11, SY10, SA11a, SSB12a, SN15, SGH10, SLZ+11a, ShMR11, Szc18, TKN13, VAT12, Viv19, WWL17, XLGA12, Xu16, Xu19, YKN13, YŠÔ12, ZE18, ZCG+17, ZL10, SP19.

MOFs [PK16]. moieties [Cha11, NCMC+18]. moiety [BS14, ELC08, SKM11]. Moiseyev [Br¨a12]. Molecular [Buc11b, CSS16, CŞSK+12, CHV14, DGR+16, DLZ11, FKBG19, FUE+12, Hor13, IIG10, KTI+12, KM12c, KKT13, MY17, MAD12, MSH13, Mar13, MP12, MOY13, McCl13a, MMT+13, MBS+18, NVI10, OHDA13, OA13, Pvs10, PWH+12, PPK+13, RAK10, SMK+12, SIT+12, SVPTM+10, SIB+13, SHS+13, SSS15, TPdMB12, UYN+13, UTtn13, VHTEG15, WML11, WVB+14, YK13, YINM13, dSDsSGA12, AC19, AV19, AS19, ABV11, BAe14, BL16, BBB+12a, BPT12, BDF+16, BMF+14, yBZfC18, BMB10, BBB+12b, BR15, BVB+18, BWE16, BH19, CRA+11, CDSK12, Cam10, CŻZI2, CTV12, CČC19, C(CL+16, CFV18, CD15, CNSK11, CHL+19, CAPL12, COP16, Dan16, DSD18, DDCY12, DI18, DMWY11, DLG12, DDF+12, DdG+11, DWGX12, Eil14, ESLM19, FZH+18, FBRBR12, FMPM+14, For12, Fra17, FK18, FBU+11, FSST16, Fuc12, FDG18].

molecular [GVPCK10, GFB12b, GI11d, GH11, GJ18, GSPR19, GR10, GHP11, GS10, HS11a, HYZS12, HYZS19, HLB19, Hii13, Hgo10, HZS14, HFL+17, HVR18, HFBC19, IFT14, IA13, IKC18, Ish14, JdL08, Jan10, KLK13, KCK14, KHH10, KKH+13, KKT14, Kry12a, KRG+13, KUY16, LB14a, LG10, Lai11, Laz14, LLM13, LA11, LTdsJ+10, LFS+11, LJSS12, LG15, LC19, LKLW11, LNI12, LB18, Ma14, Mam14, MC11b, MHT+08, Mas14, MOE+11, MMBK12, MKS13, MAF19, Mit1a, MSY+12, MVA19, MPL+11, MLB+10, MBTVR12, MBBT+12, MSAB19, MMP11, Mar12, NKK15, NDH10, NAK+17, Nic11, Nik11, NB19, OT14, OB19, OWD18, PP10, PMH+16, PH12, PBB15, Pog12, PETB18, PRG+10, Puz16, RS12b, RSM12, RBGM18, RAN18, RMC19, RP16, RLER14, Rit11, RC11, RAMB18, RdPW+12, RA10a].

molecular [SC12b, SLZ+11b, SXS+12, SLS+12, SLSZ13, Shi13, SRS+17, SACA18, SLS+10, SKY+13, SWS12, TK16a, TY17, TFA10, Tok16, TSH17, TIK13, TRZ+19, TC12, TPT19, Vik13, WZ10a, WFS13, WC14, XFW+14, XXI+16, Xul16, XWP+18, Xu19, YZHZ15, YAF+15, YT14, ZSASS13, ZFW+13, ZPR10, ZLE17, ZLWZ16, ZRLV10, ZB18, dSSF16b, dSSF16a, dOdCMUdALR11, dWLC14, dOLDLV13, vL13, vLRRK15, Puz10, RH9, RdA11].

molecular-dynamics [PP10]. molecular-level [Shi13]. Molecule [ANC+15, AM12, ASK15, Ber13c, CAZ+11, CL11, CHM+14, CHM+17, CCI11b, Cor16, DAC11, DAC12, DAR+11, DPKR12, DLG12, DCZ17, ES17, ESR18, Fra17, GWHI17, Gl11a, GT13, HK11, IIS+17, KKH18, KSC15, KP12, KN15, Lan10, LJSS12, LEU+11, Luz11b, MG11, MHT+08, MSL11, MKD19, MZLM17, MPTZ13, MJM19, MC18b, OT14, OCL+18, PK13a, RPBB11, SXS+12, SLSZ13, SLZH12, SRA+11, TFBG14, TH12, TOB19, VOAH18, Vik11a, Vik11b, WR14a, YW11a, ZZZ+18, KRC+16, TFSRM11]. Molecule-adapted [ANC+15]. molecular-TiO [TFSRM11]. molecule-to-material [TFBG14]. molecules [Agb12, Ale13, Ali19a, ACL12, AT18, BMK+14, BdTG11, BCHN16, BR10,
BAX$^{+}$19, BDG17, BB16, BB10, Cam12, CM17, CPL15, CRSB12, CKB18, CB19, CK17, CF17, DIOG12, DK13, DSRGD12, Dil13, DCR10, EML$^{+}$11, EMS16, GFB12a, GMR18, Gin10, GS11, GHP11, HRT12, HMH$^{+}$13, HST13, HNBG15, HYH$^{+}$10, HMA$^{+}$18, Jen13, JM$^{+}$X15, Jeo18, JZP17, JCCZ12, KBGC12, KBG17, KKL$^{+}$16, Kim16, KKH$^{+}$13, KKS$^{+}$11, KKT13, KKT14, LKDC11, Leh19b, Leh19c, LHX$^{+}$19, LSKM19, LPM$^{+}$11, LLP17, Luz12, MSG16, MCE11, MK10a, Mar12, May14, MFLK10, MCL11, MSM16, Mit11a, MB15, MJ11, MCK17, MPE11, Na15, NS10b, OKK10, OA13, OD16, PL11, PWY$^{+}$18, PKK14, PW13, PB10, Puz16, Puz17, RBGGM18, RGTS11, RWK$^{+}$19, RC11, Roy14, RAK10, SGB11, SD6b, SSKS12, SA11a, SKG11].

**Molecules** [SMEH15, Sha18, SB16, SMR14, SRN$^{+}$19, Sto18, SYY16, Sut12, SCZH16, SV11, THL$^{+}$15, TK16b, TH12, TXK$^{+}$19, TFMC19, Tou11a, UGWL18, VO11, XHZXXZ10, YZZ16, YD17, ZS11, ZDF13, ZP16, ZCC11, ZZZ$^{+}$18, ZS12, ZI19, dSCC12, dSTH17].

**Møller** [RS11a, BVA$^{+}$14, NMIP14, RS09, TH13].

**Monolayer** [UDS19b].

**Monomer** [Cas15, BHA19, JWG$^{+}$12, MM13, BM$^{+}$13].

**Monomers** [MBA$^{+}$13, UJSJ13].

**Monometallic** [ZW15, GZW16, ZCTG18].

**Monomolecular** [MOSK10].

**Monooxygenase** [SSI$^{+}$10].

**Monoanions** [CYL$^{+}$19].

**Monoboronyl** [MLK17].

**Monoanionic** [Bar11].

**Monobromide** [HTM10].

**Monoatomic** [DSS19].

**Monofunctional** [XZ11].

**Monofluorides** [KWC11].

**Monohalogenated** [MNV$^{+}$17].

**Monolayers** [KC19a, MDP12, RZC13, TTM16].

**Monolithic** [WWL$^{+}$11].

**Monolayered** [HTM10].

**Monte** [AF12, ABG12, ANC$^{+}$15, ASK15, Cal10, CKB$^{+}$19, CCC19, CP16, HCH$^{+}$18, Hog13, HBY14, HMI12, JCCZ12, PDR$^{+}$14, PIS18, RCGLV$^{+}$14, SGC13, SCBP17, WAG14, WCM14, ZLR15, ZCC11].

**Monomorillonite** [BJdlMAV12].

**MoO** [MFZ$^{+}$18].

**Monoclinic** [DWX$^{+}$16].

**Monodentate** [ZKKR11].

**Monooxigenase** [SSI$^{+}$10].

**Monophosphates** [PAD$^{+}$10].

**Mostar** [ACT19].

**Motif** [SLZ$^{+}$12, YD17].

**Motifs** [CJMC19, KUS19, Kry10].

**Motion** [Cam10, DLR10, KC15, KB18, MCM$^{+}$11, MMSC19, SRPD16, Sut12].
motions [HZW18, XXJ\,16, YW11a]. motors [OWD18]. moving [FAFR12].
MP2 [KBMM10, LKLW11, NMIP14, yOITn15, RSM12, SZ11, Tav12, Yu13].
MRCC [NYS\,10]. MRI [GSPR19].
MRPT2 ONBP11, SLZ\,11b, SLZ\,11a. MRI [GSPR19].
multicolor [CYLL11]. Multicomponent [STU19, GJ18, Kar13, OBP11, SLZ\,11b, SLZ\,11a]. MRI [GSPR19].
multicolor [CYLL11]. Multicomponent [STU19, GJ18, Kar13, OBP11, SLZ\,11b, SLZ\,11a]. MRI [GSPR19].
multicolor [CYLL11]. Multicomponent [STU19, GJ18, Kar13, OBP11, SLZ\,11b, SLZ\,11a]. MRI [GSPR19].
multiexcited [SCZG12]. multimode [RGPZD13]. multiobjective [SSB12a].
multiparameter [GMGRMP12, I1H16]. Multipartitioning [RS09, RS11a]. Multiphoton [NWQXi11].
Multiple [HhGqZZ17, PBM10, PP14, DB12, GFRdG11, Ish14, JW19, MGB18, NMV\,14, RWW\,19, YGLL10]. Multiple-pathways [PP14]. Multiplets [BMB16]. Multiplicative [LSW19, LWY19, PL18a]. multiplicities [Nal12].
multiply [HDÖS12]. multiply-valued [HDÖS12]. Multipole [Tal11, LBW11, YSÖ12].
multipoles [TH12]. Multireference [CYLL11, KB19, LP10b, RMG\,19, SWS12, BVP13, GSaY11, HFD11, JNZ\,14, Kon10, MdAdCS12, SYL\,18, SLZ\,11c, SZL\,14, dSM19a].
Multiscale [AHC\,18, Mas14, ZP16, CLKD15, CW\,11, MGN14, TTM16].
Multistep [SAS\,12, Sic16]. Multithreaded [MAF19]. multicolor [UGWL18].
muscinol [Ser11a]. mustard [VSMK15]. mutagenesis [CSVCB12].
mutagens [MLPT10]. mutant [dAGNJT12]. mutation [SSB12a]. mutations [DMG10, MFR10, MG10].
mutipathways [SWS\,14]. Mutual [Mat02, MAT19, Mat10]. Mycobacterium [ST15]. myoglobin [CHSO13].

N [AGOP18, BBYZ18, BJ17, CJMC19, CWS15, CSWSZ13, GC18, HWL16, JLG\,12, Kal18, LYL\,12, Men10, MC18a, OCL\,18, PCK19, Per10b, RLTTA19, SB18, SABA\,12, SSAM13, WLZ\,12a, WLZ\,12b, XXZ\,10, XXJ\,16, XCL\,18, Zha10, ZHI2, ZQFW13, SC12a, ARG11, BEM11, LL18, LWY19, YLX\,18, XWC10, ZCTG18, ABTW14, CJMC19, CTW12, CDL\,19, Est18, FLCHL10, GMM\,18, HZZ\,19, HMO10a, HXX15, KMK\,16, KMM\,18, LYL\,12, LW15, MNV\,17, MBA\,13, PRPU\,13, PL18b, Puz10, RRB12, SABA\,12, SC12a, SSAM13, SXS\,12, TMC18, Tob19, TPdMB12, WZX11, XMZ\,12, XZL\,12, XZG\,18, YLZ\,10, YWJ\,11, Zha10, ZHI2, ZGSM15, ZCG10]. N- [SC12a].
N-confused [HM10a]. N-coordinating [YZL\,10]. N-cyclic [XZG\,18].

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near-infrared [YWR+18, dARAV12]. near-IR [ZQJCJ10].
[DCBB11, KWWH18]. neglect [HVR18]. neglecting [Fe19, Na19].
nitroethylene [MLL+11a]. nested [Ca10]. Net [RLZ12]. netted [DW12].
network [Beh15, BGKK16, FCC11, MDC15, WZX15b, dAVdM17].
network-based [MDC15]. networks
[CRAC+11, CL08, LFF+10, LZZ19, MPD+15]. Neural
[BGKK16, MDC15, Beh15, CRA+11, CL08, FCC11, LFF+10, WZX15b].
near-IR [ZQJCJ10]. neuraminidase [PCF+18]. neuraminidases [YXY+12]. neurotransmitters [RZG12]. Neutral
[RFMC19, BCGC12, BGMD15, CA+11, DHYC19, EPS+16, FBRB12,
Gra11, MMRA10, ONBP11, PPSI11, RTG+19, TCM+12, Val17, ZQJCJ10].
nicotinic [CD15, Kar12c, Zaq11]. neutrons [Kar15]. newly [VVY18].
Newly [BAX+19, HMA+18, TXK+19, KRH13, LHX+19]. Next-generation
[BAX+19, HMA+18, TXK+19, LHX+19]. NH [SMC18]. NH
[AM18, yBZC18, EMSB15, MPRCEG12, WZM+13, XWCY11, XF19,
CCL+13, CRSB12, CCL+10, LV12, LLG+12, MWH15, MPRCEG12, OKR12,
RNB+10, SLZH12, SW12, XZL+12, RRVJ10, RB11b]. NH-tautomeric
[CCL+10]. NHC [Pan16]. NHC [NR+11]. Ni [AO12a, KYLC19, YL11,
AAA12, BXR+13, FBD+13, GP13b, GZMC11, Kim18, LWX+14, MRT11,
NKWT19, SFA19, SLC+18, SLZ+12, WJL+10, WRW+18]. Ni [Kim18].
Ni-loaded [LWX+14]. nicotine [PDNC14]. NiAl
[CJOOW11]. Nickel
[ASD18, LSCMSFC19, DZO12a, SDR+13, VSMK13, TFA10, dCSdMC13].
Nickel-substituted [ASD18]. Nicolaides [Ban12]. Nicotinamide
[MDP12]. nicotine [SGKJ12]. NICS [XWC10]. Nikolai [Pup11b]. Nile
[FSBA12, MRA11]. Nimrod [Brä12]. nine [PMEP19]. nitrates
[MOSK10, OB19]. nitrate [HM11, ZL10]. nitrates [HZZW11]. nitration
[LLW+11]. nitric [BGMD15, MNE+13, ONBP11]. nitride [CJMC19, Che13,
DHZS11, ES17, Esr18, FZX18, GWZ+14b, GAMM10, Ish14, TTN18, WG18].
nitride [CMCN11, NAK+17, YNL18]. nitriles [RFN+12]. nitrites [BL10].
nitro [CLY12, WGLX10, ZCC11]. nitroaniline [KC11]. nitrobenzene
[SS18b]. nitroethylene [BBAL12]. nitrogen
[BHMM19, BSO11, EAV16, EM19, GZ14, HZG12, HNBG15, KC19a, LZW+15,
MS14b, PPDF11, PP19b, RD14, VKF+19, WLL19, YZZ16, ZKRR11].
nitrogen-heterocyclic [GZ14]. nitrogen/phosphorus [BHMM19].
nitrogenase [CR18, VPOG19]. nitrogens [XxxBl9]. nitroguanidine
[DGR+16]. nitrones [AB1+19]. nitropentaamminecobalt [MMSC19].
[GR10, MJ11, RLER14, STU19, BPL13, BJ12, CG12, Cyb11, DVDBM11, FKL+12, GJ18, JHSG18, MZB+13, Mam14, MVC13, MNZPT19, NS10b, NB17, SPSA11, TMIC18, ZPM10, ZP16]. nucleic
[Kuv10, TBST10, YDW13, ZDZO10]. nucleobase [ZKWZ17]. nucleobases [CAO18, Cys11, DSVP15, KZA+17, LCH14, TD19, WG18]. nucleophilic

oligonucleotides\textsuperscript{[ACF+11]}, oligopeptide\textsuperscript{[MM10]}, oligopyrroles\textsuperscript{[DCBB11]}, oligosilane\textsuperscript{[ZYZ+11]}, oligothiophene\textsuperscript{[TZ11]}, oligopeptide\textsuperscript{[MM10]}, oligopyrroles\textsuperscript{[DCBB11]}, oligosilane\textsuperscript{[ZYZ+11]}, oligothiophene\textsuperscript{[TZ11]}.

Olof\textsuperscript{[Pyy11]}, Olson\textsuperscript{[BSS16, MSBF18]}, OMC\textsuperscript{[WCY+10]}, On-site\textsuperscript{[DLMJ14]}, on-the-fly\textsuperscript{[UTTn13]}, One\textsuperscript{[Ber13a, CG12, Dum12, LCH14, Bud12, CYK17, FCS13a, FCS13b, GTR11, GI11e, GAMM10, GS10, HZS14, Kri13, LW15, Luz11a, MSC10, MBBT+12, PVS12, RZSZ18, SC12b, SZZ+19, SWS+14, TAY11, VBC+12a, VBC+12b, WW17, WLZ+12b, YF16, ZZZ+18, TC12]}.

One-\textsuperscript{[CG12, WLZ+12b]}, one-center\textsuperscript{[HZS14]}, one-dimensional\textsuperscript{[CYK17, MSCP10, RZSZ18, VBC+12a, VBC+12b]}, One-electron\textsuperscript{[Ber13a, Dum12, LCH14, GI11e, GAMM10, GS10, Kri13, WCY+10]}, one-mode\textsuperscript{[PVS12]}, one-parameter\textsuperscript{[FCS13a, FCS13b, YF16]}, one-photon\textsuperscript{[Bud12]}, one-pot\textsuperscript{[LW15]}, one-to-one\textsuperscript{[WW17]}, one-two\textsuperscript{[TC12]}, ones\textsuperscript{[HMA+19, LW13]}, Onicescu\textsuperscript{[OH19]}, ONIOM\textsuperscript{[EFO11, EO11, KYH+13b, SKB18]}, ONO\textsuperscript{[XX12]}, onset\textsuperscript{[LB14a]}, onto\textsuperscript{[CA17, CAO18, SFW12, SRS+17, Sta10]}, OO\textsuperscript{[SBSD18, SSK+12]}, OOHH\textsuperscript{[NP18, PGG12]}, OPAL\textsuperscript{[CwCW+11]}, Open\textsuperscript{[CP16, DSM+19b, GAN14, GCK+17, HNP+12, JEA13, JH10, MAT19], NSN17, NNSN17, QSX+15, RMB18, Scha18, YMY+13}, open-close\textsuperscript{[HNP+12]}, Open-shell\textsuperscript{[CP16, JEA13, NSN17, NNSN17, YMY+13, dGr14, GXZ+14]}, open-source\textsuperscript{[DSM+19b, GCK+17, QSX+15, RMB18]}, Opening\textsuperscript{[TFBG14, AMBM+18, BAX+19, KMS+11, MBSMJ18, QB15, TXK+19]}, openings\textsuperscript{[KUTS10]}, OpenMP\textsuperscript{[WMK+19]}, Operator\textsuperscript{[DJ95, CD18, DJ12, IM15, Mys12]}, OP\textsuperscript{[DPDR11]}, Oppenheimer\textsuperscript{[BPL13, GVPC10, RSM12, Ran18, Sk17a, Sut12, VV+16]}, opportunities\textsuperscript{[FAK19]}, OPPS\textsuperscript{[ZPM10]}, opsin\textsuperscript{[TU10]}, optic\textsuperscript{[Zen11]}, Optical\textsuperscript{[LRKM10, YBMK12, AMK10, ABA11, BF11, BSM+15, BSO16, CPL15, CZLD17, DWX+16, FSQ+11, FZX18, FBU+11, GAPK+19b, GD1+10, GCGM18, GRCATG19, Hat13, HWL16, HWW18, HSS18, IGMK11, JdOS16, JFDD10, KC11, KPL+17, KL11, KMMU+13, LYW11, LZM+15, LYL+12, MFC10, MNP19, Mas14, MPJ12, MFZ+18, MA11a, MMF+13, NF+13, NMHPGV12, OGvSG18, RKM12, RRRV19, SBAT16, SSSK12, SLS+14, SM17, SYQ+10, WZL+12a, YKL11, YLW12, YHLC15, ZSQ+10]}, optics\textsuperscript{[DSRGD12, LKDC11]}, Optimal\textsuperscript{[FT15, GSP19, NVI10, NB19, TC17], YWR+18}, optimally\textsuperscript{[NTGC19, ZZ8]}, Optimization\textsuperscript{[CL08, FCC11, HJ13, KYH+13b, Kub12, Lu15, MHT+08, SCH10, SP+15, WWL17]}, optimizations\textsuperscript{[YIY+13]}, optimized\textsuperscript{[ANC+15, KPH+12, SXH18]}, Optoelectronic\textsuperscript{[AFA13, JR19, BHAH+18, KA13, MANP17, OAA19]}, orbit\textsuperscript{[Ash18, Ber13b, BDR12, CYL+18, KV19, LWL+12, MLK17, MC18b, RS12a]}, Orbital\textsuperscript{[BT15, Kon10, MM120, AOT+18, AK17, Ash18, ABA11, Bar11, CPF+11, Cn20, DVDBM11, Fin17, FA17, FMPM+14, FC19, GR10, Hog10, HVR18, IKN13, IK18, JH15, KK14a, KLK13, KCK14, Kit17, KKT13, KKT14]}.
KPH$^{+12}$, KUY16, LB18, MSNP18, MMM16, MAF19, MFLP12, MSY$^{+12}$, MAI0, Mur12, Nag15, OT14, OAT$^{+13}$, Pir13, PU14, PNC19, RMC19, SIM14, Tal11, TD11, Tsu15, XHZZX10, YPDW14, BT17]. orbital-free [AK17, Fin17, FA17, Nag15]. Orbital-Specific [MMM20, Cin20, MMM16]. Orbital [GZSMFN16, ABS11, ABS13, Boed12, CCL$^{+16}$, CFV18, CC12, DZO11, EBR11, Falk12, GZF14, GW13, GE12b, LSR$^{+10a}$, LSR$^{+11}$, Mat02, Mat10, May14, Mit11a, NZ13, Nik11, NB19, RMG$^{+19}$, RRCO11, RLZ12, SOM10, TH13, Tsu15, WWL17, YZHH15].

Order [AF16, ABA11, BR10, BR16, BVA$^{+14}$, DAC12, DCHC11, Dun15, EG10, FSQ$^{+11}$, Gin10, HSS18, KC11, KK13, KM12c, LKDC11, LCL$^{+10b}$, LPG$^{+12}$, LG12, Luz08, MSNP18, MMF$^{+13}$, NKF$^{+13}$, PDR$^{+14}$, Per10b, RL12, RS09, RS11a, SN15, TH13, UV18b, VRO$^{+12}$, WLZ$^{+12a}$, ZSQ$^{+10}$].

order-disorder [PDR$^{+14}$]. ordered [CPL15, HW12]. Ordering [GA19, AM10, GE12a]. orders [KK14a]. Organic [SA11b, WTW$^{+15}$, BF11, BDG17, BWE16, CKL16, FM16, GNM$^{+12}$, GRCATG19, HKZZ15, JPPA10, KMK$^{+16}$, KSO19, LSR$^{+10a}$, LSR$^{+11}$, LV19, LYS$^{+19}$, MUNC11, MUNZVR12, MAP$^{+10}$, MCL11, MLW16, NZAVR10, OPAM18, PFDm13, PWY$^{+18}$, PETB18, Puz17, RD PW$^{+12}$, SFL$^{+10}$, SB16, SAHA16, TCA10, Val17, WWB$^{+14}$, ZB18].

oxides

[Ali14, ASW13, BGMD15, Dau16, DLJT14, DWGX12, FSK+11, GC18, 
Hog13, KC11, LWX+14, LCH+11, MSK11, MGP16, ONBP11, Oni10, SZ11, 
TSKN12, WCY+10, XGH18a, YNLD18, YHL+13, YC13, ZDF13, ZRGE+19].

oxidized [FTB11, RRB12].

oxime [IKC18, Kan18, NAK+17, PSK+16, RGST12, RKCK19, VGGPdL19, VKF+19].

oxidoreductase [SR11a].

oxirane [BAX+19].

oxo [ZSAP11].

oxo-titanium [ZSAP11].

oxoacids [CK17].

oxoanions [HNBS18].

oxocarbon [JFDD10].

oxodithioesters [GCZ+14].

oxoguanine [YM12].

Oxygen [GLT13, SDY16, AGOP18, CAZ+11, dDGNB10, JAB12, 
KCK14, LSR+13, Mor12, MLW16, PMH+16, dSMRPF18, SCZG12, SBSD18, 
VS19, WWHZ13, YS+10, YYI+13, YSK+12, YZZ16, 
dOdCMUdALR11, OD12, YYI+12].

oxygen-evolving [LSR+13].

oxygen/nitrogen [YZZ16].

oxygenated [TYN13].

oxyluciferin [SR11b, dSdS13a].

oxypentadienyl [VGGPdL19].

ozone [ASK15, MKD19, Var14, WWHZ13, YYS15, YSS+10, YYI+12, dOdCMUdALR11, OD12, YYI+12].

oxygen-evolving [LSR+13].

oxygen/oxygen [SBSD18].

ozone [RA10b].

para [Kle11, NG11].

para-Fermionics [Kle11].

para-hydrogen [NG11].

parametric [BH19, LdMCdA+12, RSCS10, SOF+10].

parametrizations [WR15].

parametrized [Oht13].

parent [MR11, PGG12].

Papers [RA10b].

para [Kle11, NG11].

para-Fermionics [Kle11].

parallel [CLKD15, Lya19, yOITn15, PC19, SRPD16].

Parallelization [ZWSF16, MAF19].

parameterization [HSS+11, PABSK16, PSPS11, SOF+10].

parameters [AGPDZ13, AK11, BMF+14, EKN10, FV11, FCC11, SPGR19, 
IIS+17, KAR12a, LJSS12, MEG11, MPM15, MOY13, Roy16, SPO+11, 
SR11b, SWS12, WJ+17, YS+12, dCSdCMC13, dOdCMUdALR11].

Parametric [BH19, LdMCdA+12, RSCS10, SOF+10].

Part
portable \[ \text{Lya}19 \].

position \[ \text{CMR13, CJSNL11, GLPA10, MSOV13, QJ13, TTD13, VC13, Yam11} \].

potassium \[ \text{Ish}14, MMV19 \].

potency \[ \text{DKZ10} \].

potassium-iodide \[ \text{MMV19} \].

potency \[ \text{DKZ10} \].

potential \[ \text{BS18, DPPD11, OPP14, WLG11} \].

practical \[ \text{RAMB18, SIM14, SLS19} \].

prebiotic \[ \text{KS19, VFCSC17} \].

precision \[ \text{Kin13} \].

precondition \[ \text{KW18} \].

predict \[ \text{STO11} \].

predicted \[ \text{Jeo18} \].

Predicting \[ \text{ABKJ18, BPK19, DWX16, KRK17, PO15, AMMB18, CFOC10, DE18, GA19, TWR15} \].

Prediction \[ \text{DFV12, LC12, SGB11, SSP14, Ali19b, BB16, BBA16, CPL15, DGA13, GB18, LCL10b, LPG12, PCD14, PWY18, RMLPGGH16, SLC18, SRAS16, SBKJ18, VPFD10, VR012, WZX15b, XYL18, YC13, ZYSW17, ZW15, dOLdLV13, MGD11} \].

predictions \[ \text{Bou11, Bou12a, KKH18, TSK17, WLL19} \].

Preface \[ \text{ACL10, ABC12, ABo13-49, BSS14, DC10, DBMBP11, HLSD14, HB18, NYA13, NT15, Rei15, RSV10, Rup15a, RA10b} \].

preference \[ \text{EAH13, JN13} \].

preferences \[ \text{KM12b, LB18, MAW18, NRS11, NJA12} \].

preliminary \[ \text{CC12} \].

Prelude \[ \text{AS19} \].

preparation \[ \text{CS18} \].
[DPK18, DB15, EBR11, FRNM12, KSC15, Lae14, LB14b, Pit12]. Present
[TsvL+16]. Presentation [EMK14]. pressure [KMU+13, Mil12, SIT+12].
prevention [Bal16]. primary [ABKJ18, MOSK10, NGS11]. principle
[AF13, CM15, DWX+16, GI11f, KLK13, Oht13, RD14, SMGZF19, SGC13,
TCCI10, VDG13]. principles [AGG+18, BXR+13, Bon17, CC11a, CWW+16,
CJOOW11, FTB11, Fra17, GNM+12, HMA+19, Jia15, Kan17, KSS12, Kim13,
LLM13, LL16, LBqD+19, LIK15, LBdV16, LSCMSFC19, MBKH19,
MJM19, PPI19a, Per10b, RZG12, RJJPGH+13, RRB12, TZ11,
TWR15, Wan13, WLH+19, WZC+12, XCD18, YHL+13, ZWLC12, vL13].
prion [MRT11, MM10]. priori [LG10]. prismanes [GKGM18]. Pristine
[BSS15]. proapoptotic [GTSC+19]. Probability [dA12, MNZPT19, MAPS18, NTCG18, YW16].
Probable [KRH13, GI10]. probe [BAB+18, LYS+19, LGS+16, RDB18, RDB19].
probed [LSR+10a, LSR+11]. probes [GSPR19]. Probing
[GXZ+14, MA19, MRY+13, SRA+11, TWHZ14, TG13]. Problem
[DJ95, BW18, BM12, Brt11b, DJ12, DB12, DVP18, Gru17, Ign11, Ign12,
JW18, Mit11c, PFI19, RGPZD13, Rit12b, TPJC+12, UYN+13]. Problems
[LDZG16, Blo15, FRGC10, Kar10, Mar12, RMY+19, SW10, Sha18].
procedure [GTR11, KMNSP19, NS10b, Sha11a, ZS11]. procedures
[OKR12]. Proceedings [DC12, DC10]. process
[AGB19, AGRI+12, CRB+12, CL08, DWP14, GI11a, KK19, KTI+12,
LYS+19, MJ16a, MNC12, SR18, TCG17, WZX+15a]. processes
[BM10, CPAT11, KUS19, MWH15, Mar13, Mas14, PD11, RLW+13, RSL10,
Tapi15, TBHL11, TPT19, VKF+19, XZL+12, ZLWY13]. processing
[LSKM19, ZH15]. processors [Lya19]. prochiral [WTZ+11]. produced
Professor [LJ16]. proficiency [JXX+15]. profile [SIT+12, SSP14, STU19].
profiles [dHLdS12]. program [BHH+13, CYC+15, DOE+14, DCOC+19,
LCZL15, MPZWD10, YAF+15, ZHF12, ZH15, ZWSF16]. programmable
[CKB+19]. programmed [AVF12]. programming [Lya19]. progress
[HDÖS12]. progression [Ish14]. project [TY17]. projected [KSN+10].
projection [KYH+13b, Vv19]. Projector [KRC+16]. prolate [Kar12b].
proline [SHL+13, YZZ15]. proline-catalyzed [SHL+13]. Prominent
[WLC+17]. promiscuous [RNdA+10]. Promising
[LO+12, SG19, Ear18, EM19, KM12b, LYS+19, MVG18]. promoted
[LJK+18, LCM+11, PII18, QCW+12, WTZ+11]. promoting [RNdA+10].
promotion [CAPGAI18]. propagation [Bae16, EM16, KFS13, KUY16].
propagator [DZO12c, DZO12a, FMMD+10, POLV12, SM12, ZDZO10].
propagators [AMMC19]. propane [NTNL10]. propen [HNH+12]. propene
[DPFR11, ZPW16]. propensity [PSK19]. propenylamine [RJA+10].
Proper [SD13b, Fin15]. Properties [GLT13, GH11, IA13, KBF+13, KKT13,
MOY13, MC13a, ONK+13, OA13, TBRIS12, TSS+15, AGCVG15, AFA13,
AFM+10, AMK10, AMAM18, ABA11, BL16, BHAH+18, BSM+15, BGKK16,
properties

properties/activities

properties

properties

proteasome [VHTEG15, dAGNJT12]. proteases [SKS10].

protected [MC18b]. Protection [CAPGAIG18, BSS15, GA19]. Protein
[PT13, AGRI+12, CR18, CHSO13, CSVBC212, DFF+13, GSR12, HXDY16, KFY+12, KKK12, LLZaH14, MYZ+10, MRT11, MRS15, MSK+12, Pop15, TYN13, TCM+12, TBHL11, YSW11, ZP10, ZWLC12, ZT11, dA12, TBST10]. protein-coupled [CSVBC212]. Protein-nucleic [TBST10].

proteins

protic [HFL+17]. ProtNA [TBST10]. ProtNA-ASA [TBST10].

protochlorophylide [SR11a]. protocol [BDF+18, CW+11, SCBP17].

protocols [COCF+14]. Proton [SCS15, DLCB15, DLM12, DSZB18, FDMR11, IKS08, IKS10, KA011, Kry11b, Kry12b, LZ12, LYL+12, MPE15, MNC12, MGP16, NMS+10, RY12, SPPT15, SYK+12, Sat11a, Tav11,
SD16b, ST15, SLA12, TIKN11, UYN+13, VHTEG15, ZKW17, dAGNJT12. QM/MM-ER [TIKN11]. QM/MM/MD [AHC+18]. QM/polarizable [Cap16]. QM/QTAIM [BTH18]. QMMM [HCH+18]. QR [BB10, Bou12b]. QRM-SCHE-MO [BB10]. QSAR [KKM+12, MPPCM+11, PH12, XFW+14, ZFW+13]. QSPR [CD18, MPPCM+11, SN12, TFA10]. QSPR/QSAR [MPPCM+11]. QSTR [PI13]. QTAIM [BTH18, DP16, MAW+18, NH18, Shal1a, VHTEG15, XXJ+16, XWP+18, YXM+18, ZLZ+14]. quadratic [FYhC11, OPAVM18, RSN12]. quadratically [ISRK12]. quadratically [ZST+10]. quadracyclic [TTD13]. quadrilateral [LZZ19]. quadruple [MPT11, NZ13]. Quadrupole [MdAdCS12, AC11, BJ12]. quality [OKR12]. Quantal [SIB+13, SHKS15]. Quantification [SP19, Gru17, ORJ18, Rus14]. Quantifying [Mar12, MML11b]. Quantitative [CJSNL11, HSN+11, Zha17, MY17, MBTVR12]. quantities [FSST16]. quantization [HKLW13, Kle11, SD13b]. quantized [Tou11b]. Quantum [Bal16, BSS16, BL10, BR16, Bra19, Brü13, CJBMMAPR19, Cav13, CKL16, Choi16, Cho19, COP16, DKZ+10, DLCB15, DFK16, DLM+11, DC14b. EAK+10b, EML+11, EMEPD15, Ezz10, FMKJ14, For17b, GbZA10, GGZZ16, HGB08, HS15, Hog13, HB14, Hop15, IAK13, IO18, IK14, Jen13, JXX+15, KWC10, KYS13, KMK+16, KYH+13b, KUTS10, LB14a, LZZ12, Luz11b, Mak15, Man16, MMP+18b, MNE+13, MBTVR12, NTCK13, Nic14, OWD18, ÖEDB11, PH12, PWY+18, PETB18, PKK+16, PSDK17, Puz17, Qu13, RTGTS11, Rit11, RMP+14, SAG13, Shi13, SR13, SG14, ŠKB18, SBKJ18, SZY17, SSB+12b, Tap15, TFSRM11, UJSJ13, VVN+16, VBJK18, Wag14, WDSL14, WYWL13, WZX+15a, WXW+11, WCM14, WLD+10, XS18, XZJ+16, Xu16, YM12, YW11b, YZ12, YB11, ZCC11, ZJS13, dFR15a, dFR15b, dSMT+18, ASMP15, ABG12]. quantum [ANC+15, ASK15, BF11, Bau12, BAX+19, Blo15, BGL+16, BHH+13, BT15, BT17, BM16, BBS+12b, Bra10, Brä12, Buc12a, BN11, CD18, CKB+19, CM16, CS12, CSG14, CW13b, Cho15, CYK17, Coo12, CPAT11, CN12, Dau16, DP18, DSL15, DPRK12, Dil13, DMBL16, DSFT17, EAH13, FLCHL10, FBO+11, FNIT16, FSST16, Gag11, Gan14, GWZ+14a, GRCGRRHT19, GB10, GSI1, GR10, HR13, HS11a, HITU16, HS1c, HEVMSA+19, HM12, Hor13, HMA+18, IFT14, Ish14, JN13, JHSG18, JMX+15, Kap12, KB12, KCDC15, KC18, Kar09, Kar10, Kha16, KCC13, Kit14, Kit15, Kle11, KN15, KK11d, LS17, LSS19, LV19, LSR+13, LCZL15, LHX+19, Lin14, Liu15b, Liu16, LSKM19, LEU+11, Luz11a, Ma14, MC11a, MR12, Mam14, MDC15, MEP15, Mar13, MSC10, MML+16, MPD+10, MQG13, MPL+11, MBBT+12]. quantum [Mor13, MLDP10, MB12, MGP16, NC11, NKKN15, NS10b, NGS11, NBZG16, Ném14, Nic1, NVPCJ+13, NMSR14, NRP+11, NJA+12, Nym14, OPS10, OK19, OMT13b, OSJ+12, PABSK16, PTH11, PMGMGR12, PMHM19, Pup11b, RP11a, RP11b, RL12, Rei15, RDM+11, RNE10, RNB+10, Rup15a, Rup15b, SDS19, SDS20, SOF+10, SBEH11, SKHN13, SC12a, SPSA11, SN15, SK17b,
SKLC19, SD13b, Sha18, She13, SIB+13, SHKS15, SKM11, SSA18, SGC13, Sjö15, SS19b, SYF12, SRA+11, STU19, SZ15, SCBP17, SPM+15, Tch13, TBB+19, TK16b, TH12, TXK+19, TFA10, Tri14, TB15, UTT13, UV18b, VPFD10, VMR11, VVVB10, Vik11a, VOK+18, VO12, WYM15, WR14b, YNL18, YÇÖ11, YZ13, YW18a, YS13, YH14a, YW16, YLC17, YLYC18, ZS11, ZX12, ZGSM15, ZHI15, ZWSF16, ZZC12, ZWE12, ZRLV10, dHLdS12].

quantum [dSTH17, vLRRK15, AGNS14, BMRM19, DMS+10, GP13a, SP19, ZBK15].
Quantum-chemical [DLM+11, ÖEDB11, Qu13, BF11, DMBL16, DSFT17, MGP16, Ném14, NVP13+13, SN15, VOK+18, YNL18, DMS+10].
Quantum-chemical-aided [GbZA10].
Quantum-classical [Cho16, Cho19, Mak15, SPSA11].
Quantum-matter [Tap15].
quantum-mechanical [LV19, VPFD10]. quantum/classical [CP11].
Quantumness [CD15]. quartet [HK11, SCZG12, ZCG10]. Quartic [VBC+12b, FT15, dAB17]. quartz [LLM13].
[BAP12, BGL+16, DLG12, JEA13, JMP19, LWL19, MURR13, SZZ+19, TMC18, YJ17, ZQCJ10]. rare-gas [SZZ+19]. Rashba [KV19, SBD+16].
Ratchet [BEPZ10b]. Rate
[WZH13, AFM+10, Buc12a, CAIA12, CGIA12, DCO1+19, FLCHL10, FM+10, MVC13, MIKH19, NZLG15, dMOB12, ZLWL16, ZXY13, SSP14]. rates [AC11, CCM08, RFEGPP+16, YK13]. Rational [LLZ+14, WR14b].
rationale [JWJ+12]. rationally [LLZ+14, WR14b].
Rayleigh [BDR12, MB12, dSCC12]. Rb
[ˇCFˇC11, DIOG12, MLW10, RBTL19]. RbH [KHH10]. RbSi [LHL+15].
RCOOH [DQZF12, NBL12]. RDC [PT13]. RDM [KK14a]. RDX
[Jeo18, MJ11, TJ17]. RDX- [Jeo18]. Re
[BvWG14, Kaw15, LNGW14, NZLG15, SKS10, SR18, VPG12, WWLZ17, ZSHL16, ZP16, ABM+19, AGOP14, lAy14, AG10a, AG10b, AASU+17, AEAS+19, AGNS14, AFM+10, ASD14, BPT12, BAMA12, BZZ15, BLJ17, BZ+19, Buc12a, CLKD15, DS12, DAA16, DPDR11, DZ11a, DSZB18, EHD11, EM17, EHM+10, EDA16, FLT14, FY17, FUE+12, GWZ+14a, GZFM13, GKT+12, HSS+11, HX15, HHL+12b, HhGqZZ17, Iku17, IK14, JW+12, JAB12, KAR12a, KI15, KI12, LGM+18, LKOS17, Les12, LZZ12, LZFZ13, LLP+13, LW1Z13, LD17, LZ+18, LFT18, LS19, LLC+11, LCH+11, LW+10, LSW12, LSG11b, LCL+11, LWW13, LWW14, SWS+14, SZ15, SY17, SHMR11, TM13, TSL11, Tsn15, TGA+11, WXZ+11, WWZH13, WX+11, WJ11, XGH18a, XZL+12, XDM+10, YKL12, YNL18, YY18a, YK13, YGL+11, YZ10, YLC18, YLFC18, ZRG+19, ZZ11, ZH12, Zha14, ZLWL16, ZCG+17, ZYSW17, ZWL18, ZPB12, ZXY13, ZSS+13, ZJC+13, Zil14, dHLdS12]. reaction-field
[SHMR11].
Reactions
[KKH+13, LLM13, MNE+13, OD12, TIN13, TM13, ACR10, AMMB+18, BRS10, BS14, BAX+19, Buc12b, CdAFS+12, CM12, Chr10, CJGT12, DWZ11, DAA16, DFK16, EMED+12, EMEP15, FNM12, FDMR11, GGG16, GB18, HDC+11, HL1Z11, HB14, Hop15, HX15, HCL13, Kan11, KZZ13b, KMM16, LJK+18, LW11, LLF17, LGW11, LSG+14, MHC18, MIKH19, MAP+10, MBSMC18, NW19, NAK+17, dMOB12, RLW+13, SCH12a, SHS+13, SKM11, SWS+14, TFZ+15, Var14, WLG+11, WLWT12, WZ1H13, WLWL14, XLZ10, YSS+10, YS18, ZGSM15, ZXY13, ZQXP17]. reactivated [MG10]. reactive
[Cho15, dDG10a, RCM+19, RL12, Ser11b, XCD18]. Reactivities
[YM13, LLLZ10, MDNO+16]. Reactivity
[JS18, KSC15, OPF11, PMH+16, TWHZ14, TV13, BVRM10, Cha11, DVC14, DNCKCS+12, ESBVJY12, GFPV19, GTSC+19, GGP13, HMA+19, HR19, Hg13, JWJ+12, KP10, KO14, MMM12, MUNZVR12, MAP+10, MBA+13, MBBT+12, MBSMJ+16, MCRR16, NAK+17, NE11, NZAVR10, OPAVM18, RGS+13, RBLZ15, RBT19, SMZ19, Ser11a, SC10b, TM19, WJ11, YSK+12, YXM+18, RdA11]. **reagent** [BPT12, LWZW13]. **reagents** [VOK+18]. **Real** [GKT+12, HR13, Fin14a, FNIT16, GI11b, GI11c, PI16, RLRI13b, SHKS15]. **Real-time** [HR13, FNIT16, PI16, SHKS15]. **reality** [SPSA11]. **Realization** [PM12]. **realistic** [SMR14]. **rearrangement** [SKS11, WTH11, YY18b, ZAE10]. **rearrangements** [WCGD12]. **rearranges** [MG10]. **reason** [PWP+18]. **ReaxFF** [BGKK16]. **recently** [JPPA10, TCA10]. **Receptor** [KKM+12, CRSB12, CSVCB12, MSY+12, SSP+17a, SK11, SKB18, WTH11]. **receptors** [PRG+10]. **recipe** [STM18]. **recognition** [Cav17]. **recognitions** [YWY+12]. **Recognizing** [Cav17]. **recombination** [BMF13, dMOB12]. **reconstructed** [dLdOdAD12]. **Reconstructing** [YS13]. **reconstruction** [AST19, GD11]. **reconverge** [Lun13a, Lun13b, MPD+15, Tou13, YMY+13]. **recurrence** [HSN18]. **Recursion** [LYW13]. **recursive** [SMR14]. **red** [FSBA12, Kry10, MRA11]. **red-** [Kry10]. **Redox** [MLY+16, AC19, AGJ12, BBA+16, ESS13, KB13, KRK+17, LCH14, VLG12]. **reduced** [ABL12, CM15, KK13, Lat13, MPE11, Per18, dCGAMV12]. **reductase** [SDM12, SLS+10, TSK12]. **reduction** [AGOP18, Esr18, KGK13, QCW+12, SBS18, VPOG19, WTA+11, YHL+13]. **reductions** [Srl18]. **reevaluation** [GI14]. **reference** [NS13, NF11, SBK18]. **refined** [SYK+12]. **reflecting** [AA11]. **reformulation** [Lev10]. **refractive** [SHMR11]. **Regina** [HS15]. **regio** [CM12, GHCMCMQ17]. **regio-** [CM12]. **regio-selectivity** [GHCMCMQ17]. **region** [EMED+12, KYS13, OVT+16]. **regional** [NGS11]. **regions** [LdBF+12]. **regioselective** [iku17, LKZ+16]. **regioselectivity** [DPDR11, DM0W11, NAK+17, YNL18, Zha15]. **regression** [VSL+15]. **regular** [PR10a, Pal10]. **regulated** [MBA+19]. **rehybridization** [Sch15]. **REIN** [MR15]. **Reinvestigation** [NRH11]. **relafen** [YNM13]. **related** [Buc12b, HNH+12, Kal18, Luz13, MSAB19, RALK18, RLY+13, SSI+10, TD11, TFMC19, UMS13, VLG12, WVL14]. **Relation** [PM16, HSN18, KM12c, RBGGM18]. **relations** [AEÖ12, DB13a, GZSMFN16, LWY13, OOM+19, RS13]. **Relationship** [CJZ12, DNCKCS+12, GXZ+14, Gra08, Gra11, LB1V16, MY17, RGST12]. **Relationships** [NBI+10, CJSNLM11, EKN10]. **Relative** [SFW12, BMX+19, LNV+18, MC17, Pan16, PSKV19, ZSZ14]. **relatives** [Fin14a]. **Relativistic** [BCK19, Fri12, Liu14, MM19, RLTAT19, SH18a, CSG14, DAC12, FSST16, GAPK+19b, Leh19c, MGGCM+19, MPTZ13, MZT16, NS17, NNSN17, OCGM+19, RR19, RTT10, SN15, SS12, ZE18, ZKKR11, ZQXP17].
rotation [Å12b, CPL15, DDF+12, HK11, HRT12, KKB17, QD10, Sut12].
rotation-vibration [HRT12, QD10]. rotational
[AEO12, CCBR+12, DCR10, Puz17, RMJJ1, SPO+11, VLM+10]. rotations
[JdOS16, KMS+11]. rovibrational [PBB15]. route
[BMF13, HGBO8, SRS+17]. routes [VPGC12]. Rovibrational
[LLP17, AM12, FT15, VLF12]. rovibrationally [Dan16]. row
[BZBZ13, KWC11, MKM11, ZFC+17]. RPA [LZ10]. RRKM [DS12, STL12].
RS [ESS13]. RT [KKG12]. Ru
[PP19a, MJ16a, OG19, SG19, YTY+12, ZPW16]. Ru-catalyzed [ZPW16].
rubidium [LHL+15, MMR+10]. rubidium-doped [LHL+15]. RuCl
[CCL+10]. rule [DMWY11, JL12a, KT12a, MHT+08, MC18a, SD13b,
XWC10, YLY+17, KKS11b]. rules [RBGGM18]. Rung [Jan13]. Russian
[Tch16]. ruthenium [ADR+18, CBW+13, DFC17, HJKD11, EKD12, GZW+14a, KMS17,
Kin13, LJK+18, MEEA+13, OD12, PCK19, PIR18, TCD12, Tan13, TL15,
WYL13, XHZXXZ10, XXJ+16, YXM+18, Zha14].
S-adenosylmethionine-dependent [WYWL13]. S-doped [OGvSG18].
S-nitrosothiols [XHZXXZ10]. S2p [LdbF+12]. S2s [LdbF+12]. saddle
[QB15]. safety [FUE+12]. Sahni [VUC13]. salen [TMM+14].
salicilidemethylfurlyamine [GW18]. salt [CLMY12, RMTG11].
salt-bridge [CLMY12]. salts [Bon17, BM10, LG15, LMCZ11].
sampling [BBB+12b, SKV12]. samplings [BS16]. Sanderson [SMGFZ19].
sandwich [DZ012b, LXD13, WCY+10, YZW15b]. sandwich-like
[WY+10]. sandwiches [SSB19]. Sanibel [ÖS12b]. Santos [HS15, dFR15a].
SAPO [SACA18]. SAPO-11 [GSB10, SACA18]. SAPT [JNY17]. sarin
[GZSMFN16, GZSMFN16]. SBO-3G [GZSMFN16]. scaffold
[OSJ+12, ST15]. scaffolds [TFZ+15]. scalability [CKYR18]. scalable
[CKB+19]. scalar [HEVMSA+19]. Scale
[Lya14, CKYR18, DFF+13, RMB18, SN15, SKV12, ZLY13, MBTVR12].
Scale-adaptive [Lya14]. scaled [YF16]. scales [DP11]. scaling
[DB13a, DVP18, JHI13, KJ16a, KJ16b, Kri13, LCL15, QX+15, RCP14].
SCAN [KME+18]. scandium [BBY18, GGD13, XCD18, OH13].
scandium-based [BBY18]. Scanning [ZLWH13]. scarce [SG19]. Scarf
[QD10]. Scattering [III16, A15, CD15, Choi15, CYK17, Choi19, Kar12c,
Kar15, NA14, RL12, RW11, SY10, SSA18, TBSTM12, Zal11, ZH15, dSCC12].
scavenger [GAI19]. scavengers [MG18]. scavenging
semiconductor [DLJT14, Fer11, KP11, Kar12b, SAHG11, VVY18].
semiconductors [BWE16, Eng16, HKZZ15, WDS19, YHL+13].
semiregular [Bib13].
Sensing [NEEV15, IKC18, Man16, MBSAG16a, MBSAG16b, dSMT+18].
Sensitized [AGJ12, BDG17, FM16, cLqFtW+14, MY17, MANP17, PMAP12, QJ13, SG19, SS515, WWB+14, Zha17].
Sensitizers [CWB+13, LGS+16, SG19, SSS15].
Series [CLMY12].
Serine [CLMY12].
Serotonin [CSVCB12, CSSK+12].
Serrano [Mer11].
Serrano-Andrés [Mer11].
SERS [TSBSM12].
Seventh [NYA+13].
Several [Tch16, MMM+12, SLSZ13, XZYS10, YY+13].
 Sextet [AM12, RB18].
 Sextuple [SLZ+11a].
 SGSA [SOF+10].
 SH [BDF+16, BXZ+19, CdAFS+12, dSNBG08].
 Shannon [BW18, Bar11, Gan14, KdSm+10, KFJ+18].
 Shape [CL18, NMV+14, BXR+13, BVP13, KP11, LKN13, SSAM13, XWCY11].
 Shape- [LKN13].
 Shape-Inducing [PN11, KKH+13].
 Shapes [IROW10].
 Sharing [BBKO16].
 Shcl [MZLM17].
 Sheet [BHAH+18, SJW13].
 Shell [CP16, Fin14a, Fin15, GB17, GXX+14, JEA13, JMPI19, KK13, DVLC19, LSC+18, MSRu+11, NNS17, NNSN17, PJ19, STM18, SDY16, SX18, YMM+13, dSDS13b, dGR14].
 Shell-Confined [SJ19].
 Shell-Inducing [LSC+18].
 Shells [GHP11, PUF+11].
 Shielding [Cyb11, MKG+11, NB17, RRK16, SS12].
 Shift [Bou11, Bou12a, LCB10, MFB11, Rit11a, Rit12b, SCB+14, SK10, TKSK17, XGH18a].
 Shifted
shifting \cite{dOR10}. shifts \cite{CRSB12, CFGC11, FBD+13, RR19, Tap15}. SHN \cite{NRP+11, SS11}. short \cite{Dum12, GST11, NWQX11, RMC19, SB16, WWL+11, XCD18}. short-living \cite{SB16}. short-loop \cite{Dum12}. shortcomings \cite{MGN14}. should \cite{She13}. showing \cite{DSH18}. shuttle \cite{Ali19a, FDMR11}. SHX \cite{EMSB15}. Si \cite{GLF+12, JL12a, MGD11, TW10, VPFD10, XCL+18, ZHL+19, CN12, ENV15, Esr18, GKG18, LKN13, LBY+14, LW18, LLLB13, MGP10, MBA+13, MSVCI10, OD16, PWL+10, WLWL14, ZCX+16}. Si-[ZCX+16]. Si-doped \cite{ENV15}. SiC \cite{LXLL11, TCCI10}. SiCH \cite{FT15}. SiCNT \cite{SD16a}. side \cite{DSCO+13, MPE11, NHG+12}. side-chain \cite{DSCO+13}. sieve \cite{SACA18}. SiF \cite{KMM16, KMM16, SLS+12}. SiGe \cite{LLLB13}. Sigma \cite{DAC11, FC19}. sigma/pi \cite{FC19}. signal \cite{GSPR19, QZH13}. signature \cite{GDM+10}. signatures \cite{BR08, BR12a, RB08, RB11a, SCL19, ZR13}. signed \cite{SK17b, SKLC19}. Significance \cite{Chu12, ELC08, Kut10}. Sigma \cite{HCL13, RLW+13}. silica \cite{CRSB12, SFNC+18}. silicate \cite{Ped16}. Silicene \cite{WLH+19}. Silica \cite{COP16, HS15}. silver \cite{AMK10, Boe12, BPK19, RFMC19, SS18b, YJ17}. silver-ligand \cite{BPK19}. silapolymer \cite{TYL10}. silica \cite{CRSB12, SFNC+18}. similar \cite{BB16, MK10a}. similarities \cite{ART08, Luz11b, MBTVR12, MBBT+12, Sat11b}. Similarity \cite{QBRA18, BM16, DCR10, Fin15, FB17, KV11, Lev10, LPM+11, MA12, MT10, SAS+12, SGL+16, SGG12, STM18, SLS+19, Szc18, TLC+17, TC12, VSL+15, YZZ+16, ZT13, ZDF+13}. Simplification \cite{CFOC+10}. Simplified \cite{GZF14, GZSMFN16}. simultan \cite{HYZ13}. simulate \cite{SKLC19, SKV12}. Simulated \cite{TGC17, VVS+18, AM13a, Eil14, JPP+11, MOE+11, VVN+16}. Simulating \cite{DMBJ15, GMA+19, MRS15}. Simulation \cite{LPM+11, CW+11, CSK12, CS17, CTDOLA10, DKZ+10, DGR+16, DLZ11, FFF10, Fra17, FNT16, GW18, Hog13, IFT13, IFT14, Kim19, KST12, LCT14, LL17, Mas14, MDP+10, MPZWD10, MG12, NKK15, Net12, NDM+12, PP10, PMH+16, SLS+10, Tan13, UTThn13, YAF+15, YT14, YIN13, ZWSF16}. Simulations \cite{Hor13, MSH13, Mar13, OHDA13, SIB+13, SLS+13, UYN+13, UTThn13, YK13, ÁFV+12, AF19b, ATS15, BMF+14, BM10, CLK15, CKY18, GPVPC10, GSR12, GSPR19, HFBC19, IKC18, Kit15, KKH+13, KFS13, LFS+11, MGN14, MM10, MMT+13, MBS+18, PDR+14, Pha19, PIS18, PP+13, QXS+15, RP16, RNC+14, SHKS15, SBL11, TGRP19, TSH17, TPdMB12, UV18a, ZWLC12, Zha17}. sinc \cite{KRC+16}. sine \cite{dAB17}. Single \cite{Esr18, Sri18, Bar11, Bas11, DI10, DCZ17, ETGLMJ+19, EM19, Fra17, HNBG15, KG08, LZZ+11, DVMC19, MR12, MSOV13, RLZ12, SD13a, SD16a, SVPTM+10, SWS+14, TKS11, TC10, XGH18a, YW16}. Single- \cite{Sri18, DVMC19}. single-electron \cite{LZZ+11}. single-molecule \cite{Fra17}.
singularities [SKG11]. SiO [DCDD10]. Siroheme [SDM12].
Siroheme-containing [SDM12]. site [AO12a, BGFD14, DLJT14, DPRK12, KRH13, KSY+11, MS10, OH13, PK13a, SKB18, SZ11, TOSN12, TSKN12, TYN13, WH18, XCD18, dCDC+11]. sites [ATL+14, BSO11, LKd+16, OPF11, QZH13, RDB18, RDB19, Ser11a, Ser11b, SACA18]. situation [CPF12]. Six [Nes10, BBKO16].
six-membered [BBKO16]. Size [MW15, BHAH+18, BGL+16, GWZ+14b, GI10, Kar12b, LKN13, MPMCM+11, WLZ+12a, ZRY+13, RS09, RS11a].
Slater [FB17, GZF14, GW13, Hog10, JH15, RLER14, RVO+14, RRCO11].
Slater-type [GZF14, GW13, Hog10, JH15, RVO+14, RRCO11].
solubility [RGS+13]. soluble [GLPA10]. solute [Cap16, MFB11]. solutes [Cam10, RTG+19]. Solution [KC16, AMMK11, ATPR11, BKM15, Bra10, BCF+11, Cam12, DE18, DCOC+19, FPRGMHB12, GCDNNS12, HS11a, HR12, HFD12, ILBS10, KS11, Kha16, LLP+13, LGZC15, Lu10, MSH13, MK10b, MPE15, MB14, QSX+15, RZZS18, RZG12, RP16, RCM10, RW12, Rit12b, SL10, SM10b, WXB+11, Zag11, ZKWZ17, ZH19, DM12]. Solutions
[FKBG19, AEÖ12, EI11, HYZS12, HYZS19, LDZG16, LEU+11, PS10a, PVS11, PVS12, PT13, PGMRGM15, RMLPGGGH16, SMV11, SCL19, TIKN11, ZLJ11, ZHF12, ZPZ15]. solvable
[GMGRMP12, Kuhb12, PGGRMP10, PMGMGR12]. solvated
[CLMY12, GMA+19, HFBC19, LCCH11, LSKM19]. Solvation
[GLPA10, MSK+12, RTG+19, AM18, BH10a, Car19, DMS+19b, FAK19, JCC10, Li15, Owel17, PCR+11, RFN+12, SL10, SLS+19]. solvation-layer
[RTG+19]. Solvatochromic
[LCB10, MFB11]. solvatochromism
[Men15, MR˚A11]. Solvatofluorochromism
[FSBA12]. solve
[Blo15, CRA+11, Ign11, Ign12, Kri13]. solved
[SW10]. Solvent
[CCC19, EKD12, HR19, RdA11, RMTG11, dAVdM17, AGOP18, BS11, Cap16, CYLL11, CS17, DLO16, DFF+13, GZF13, HFL+17, IG11k, IK14, JN13, KI15, LJK+18, LWL10, LWJL10, LDW+11, LLZ+12, MG12, MKHM11, QHS11, SN12, TC10, WLD+10, XX12, XWC11b]. solvent-separated
[LJK+18]. solvents
[COCF+14, HFL+17, KP10, MIKH19]. Some
[Brå11b, Jou13, Luz12, SW10, Sha18, Sut12, VATPR11, ZYL+14, AF16, AMAM18, ALB18, BCGC12, DCR10, EAK+10b, EAK+10a, E11, For12, GCNGS12, GB10, GI11b, GI11c, HS11b, KCC13, Kin13, MANP17, MIKH19, MAP+10, PL11, Pie12, Roy13, SGL+16, Tch16, TCA10, VO11, XHZXXZ10, ZCC11, ZLZ+14, ZZC12, Sic16]. SOS
[RNC+14]. SOS/QM/MM
[RNC+14]. soundness
[Sha11a]. source
[DSM+19b, GCK+17, Hor13, QSX+15, RAMB18]. sources
[LtdSJ+10]. sp
[She13, MCK17]. space
[BVP13, BGBV12, CDT12, Fin14a, GRD11, HN12, KPH+12, MSNP18, MFLK11, MQA17, Na12, Na13, PC16, RW12, SH19, SHTI15, SBL11, VMR11, WWL17, Ze18, vL13]. spacers
[ALRAE11, KI14a]. spacetime
[Bi13, LSW19, LW19, LZZ19, PL18a]. sparkle
[FS11]. spatial
[ABP13, CDS+18, GKM18, Pit12, RBL19, SR12]. Spatially
[AT18, CK18, GFZ14]. Special
[AH19, ÁJGVZW12, For17a, LV16, NYA+13, NT15, ÖS12b, Rei15, Rup15a]. speciation
[HFL+17, RDB18]. species
[APK+19a, GS11, HJK013, Kal18, MGD11, RFMC19, SSI+10, SM14b, SM14c, SM14d, SM16, SBSD18, YHLC15, dHLD15]. Specific
[MMM20, Cin20, LZZ+11, Lya19, MMM16, MSY+12, Nic11]. specificity
[PS10a]. Spectra
[Mly+16, AEKGZ12, AFC+10, ÁFV12, AEM+12, Ban12, BBB+12a, BS11, Ber13b, BBB16, BBAL12, BKPK19, CP10, CFP+10, CHH+19, CS17, CML+16, CLMY12, DSH+13, E114, FBO+11, For12, GI12, GKM18, ILBS10, IHG10, JPPA10, JPP+11, KV11, KBBM10, LYW11, LWL+12, LMZ15, LLP17, MC11a, MPJ12, MSK11, MAA13, Mor13, NBI+10, OVT+16, ORJ18, PR10a, PCR+11, FJP10, RNC+14, SBAT16, SB10a, SPO+11, SZZZ11, TZ11, TFSRM11, TT10, TG13, VPDF10, VVS+18, VSN+11, Zen11, ZQCJ10, ZWL12, ZLE17, ZSZ14, ZQXP17, ZI19, dARAV12]. Spectral
[LLH15,
Mys12, CdLdSC18, FBU+11, KP12, KM19, LYR+17, SMGZ13, XLZ+19. spectral-luminescent [KP12]. Spectral/structural [LLH15].

spectrometry [ABKJ18]. Spectroscopic [BH10b, Jac12, Mag14, NC11, NVPCJ+13, SZS+10, SLZ+11c, SLZ+11a, SLS+11, XSS+12, SLS+12, WFS13, BD12, CHM+14, CWB+13, CJOOW11, DAE+12, GFB12a, KSSK16, LJSS12, LZZ+17, MG12, MPTZ13, QHS11, RNdA+10, Sch10b, SYL+18, SLSZ13, SWS12, Tas14, VLG12, VLFG12, VBO+15, WXB+11, YZL+10, YZL+11, ZLJS10, ZR13, dSDSPG11].

Spectroscopical [MSBF18]. Spectroscopies [KKT13, MOY13, McC13a, OA13]. spectroscopy [Ber13a, BDR12, BWB+18, For17b, GFB12b, LdBF+12, Mas10, MML11b, ORJ18, Ped16, Puz17, SA11b, UTTn13, YJ17, ZPZ15, RdA11].

spectrum [AA11, BS16, BDF+18, BBB+12b, Bou12b, CWF11, CRSB12, DSD18, DHZS11, DWGX12, HHCA10, HRT12, HMH+13, HYH+10, JCC10, KBG17, NDM+12, QD10, RS12a, SBKJ18, WWC17, Zha17]. Speculation [KRH13].

spent [HB14]. spermine [SGB11]. Spherical [Kit15, PML+11, Roy15, CH17, CB19, CN12, GAPK+19b, Nik11, OHDA13, RLR13b, RAFL18a, RAFL18b, Roy16]. Spherical-harmonics [Kit15]. spherically [JZZH17, Nag16b]. spheroconal [MFLK10]. spheroidal [OPC17]. Spin [BDR12, DCDG10, JR12, Kle11, Luz11a, MLK17, NKWT19, SAHG11, SAHA12, Swa13, YLY+12, ATL+14, Ash18, Ber13b, Bla15, Bra10, CR18, CCP18, CYL+18, CFGC11, CSP+10, CDT12, DS11, DM16, FSST16, GXZ+14, GLXL18, GFRdG11, Joh17, Kap12, KK14a, KV19, KSN+10, KYH+13b, LVdSM14, LWL+12, LB19, Luz12, MR12, MPRB+10, Mos14, MC18b, NSN17, NNSN17, OS10b, PBR18, Qu13, RS12a, RLZ12, SR12, SRASZ16, SSP+17b, SBD+16, TÁ10, TD11, Viv19, WH12, Yur13, Yur15, ZSQ+10].


Sr-doped [Oni10]. SrBi [HLMO11]. SrC [ZFW+13]. SrH [HMI+15]. SrTiO [OH13, WCL+17, OH12]. SS [SZZ+12]. SSH [DTFK15]. stabilities [AF16, MS17, SFW12, SUL+11, SM14c, ZYL+13, dAVdM17]. Stability [GV11, KZA+17, Kry11b, LWL19, MC12, PMEP19, TLC+17, USL+13, BMX+19, Boe12, CCC19, CYL+19, CWSZ13, DVC14, FBRBR12, GJ18, GB13, GAMM10, GWJ12, HLB19, Ire12, KK11b, Kry12b, LGHL11, LCZ15, LGS+16, MNV+17, MC17, MCARL11, MMW19, MJ14, MMV+19, MM10, MS14b,
Structuring [KRG+13]. studied [AMMK11, BL10, CK17, DCHC11, FBO+11, SJZ+18, TTM16, ZL10, dSdS13b]. Studies [PCF+18, Roy13, ACF+11, AMK10, AVG19b, BD12, Buc11b, CJBMMAPR19, CCA+12, ÇAS13, CYLL11, CTW12, CWB+13, CSVCB12, CSSK+12, DSWL11, DSZB18, DB15, EAK+10b, EI11, For12, GGD12, GKT+12, GZBH18, HTM10, HNBG15, Hop15, HWL16, JL12b, KDC+12, KMM+18, KA13, KSY+11, KAOB11, Les12, LWL+12, LSR+13, LBY+14, LGZC15, LWJL10, LKLW11, MANP17, MLPT10, MAP+10, MMY+12, MSAB19, NTCK13, ONBP11, ÖEDB11, PBM10, PTD+12, PETB18, PAPCMM+16, RJY+10, RJIA+10, RTGS11, Rnda+10, Rii10, Riv11, RGS+13, RGR12, Roy14, SMK+12, SC16a, SJZL12, SIS+08, SK12b, SZ15, SSB+12b, TIKN11, TOSN12, TYN13, TAY11, Tan12, TIN13, TXL10, THSR13, UJSJ13, VGGPdL19, VPOG19, WZX11, WTH+11, Wan13, WZM+13, WYWL13, WLH+19, WHM14, Wit18, WWGW18, XS18, XFW+14, YZL+10, YZW+15a, YB11, ZZL+11, ZZX10, ZYX+11, ZQJW13, ZLWY13, ZLZ+14].

studies [ZWL18, ZSZ14, dAGNJT12, YWY+12]. Study [Bar11, BWB+18, CH17, CYL+18, IFT13, IFT14, SGL+16, SS19b, ZCP11, AC19, AFC+10, IayL14, AM12, AASU+17, AEAS+19, ATM17, AKC10, ASW13, AVG19a, ASD14, AMAC12, AG19, BMK+14, BD14, BF11, BCCG12, BDF+16, BDF+18, Bas11, BAMA12, BB18, BLR12, BS11, BEM11, BBZB13, Ber13a, BL11, BLRdA+10, BHAH+18, BS14, BSSS19, BZZ15, yBZc18, BXZ+19, BDG17, BLdV19, BMF13, Bon17, BGJSM+18, BDR12, BCF+11, BPSM12, BLM+12, BJ17, BJdlAV12, BTH18, Buc10, BO11, BVRM10, BC+12, BB16, BS12, BSK11, CRB+12, CMR13, CAZ+11, CLXZ12, CLL+13, Cao17, CPL15, CPF12, CCBR+12, CHM+14, CHH+19, CC12, CW16, CM12, CCL+10, Che12, CCS13, CWW+16, CZLD17, CLY12, CS13, CWS15, CZZC19, CK13, CFGC11, CGIAI12, CAPL12, CPAT11, CJOOW11, CD12, CS18, DWJZ11, DCCB11, DIOG12]. study [DMAB12, DAR+11, DDS18, DS11, DPK18, DS12, DC16, DSRGD12, DPRK12, DPRD11, DTEMK11, DZ11a, DLO16, DG19, DMS+10, DCdG10, DDF+12, DdG+11, DQZF12, DWGX12, DSH+13, DCR10, DFT17, DFF+13, EG10, ESD016, ELCO8, EAH13, EFO11, EO11, ETGLMJ+19, EBH11, EA12, ENV15, ES17, ESR18, EM19, ESBV12, FSO+11, FZX18, FFF10, FO10, FM16, FTB11, FRNM12, FDN10, Fni14a, FT15, FPRGMHGB12, FBU+11, Gag11, GBS17, GWM11, Gao12, GLF+12, GGJD13, GZW16, GHGF12,
GK12, GLXL18, GIO12, GFB12b, GC18, GP13b, GMT16, GMT18, GS11, GLOGM+11, GHCMMCMQ17, GB18, GWME18, GD11, GSB10, GT13, GTSC+19, GGP13, GLPA10, GCZ+14, HNH+12, HMA+19, HK11, HTC+11, HJZ11, HZL+14, HZZ+19, HDF11, HHL12a, HHL14, HM12, HM10a, HKLW13, HZZW11, HFL+17, HHL+12b, HhGqZZ17, IWI+11, Iku17, IGMK11.

study [IM15, JPPA10, JN13, Jali10, Jan10, JB18, JS17, JCCZ12, JSLH14, JLZ+17, JB11, JWG+12, JFDD10, KM12a, KS11, KWC10, KWC11, KP11, KBF+13, KKM+12, KI15, KI12, KK14b, KSAK17, KZZ13a, KZZ13b, KUTS10, KKT13, KKT14, KG08, KO12, KMA+13, KK11d, KBMM10, Lan10, LGM+18, LLM13, LKOS17, LKJ+18, LVDsdM14, LPOP12, LZZB10, LCL+11, LJL+11, LW11, LNW+11, LYN11, LGP+11, LMZ+11, LGP+12, LLP+13, LXW+14, LL11, LYT+17, LFF17, LZW+18, LTL18, LFTL18, LW+11, LLC+11, LGW11, LLLB13, LLL+17, LLF17, LD17, LZW+18, LTL18, LLW+11, LLC+11, LGW11, LCZ15, LL19, LCH+11, LSL12, LW+12, LWZ+14, LL17, LLW+12, Lu10, LWC+10, LCS+11a, LCH+11, LCS+11b, LXLL11, LLLB13, LW13, DVMC19, LKZ+16, MYZ+10, MLW+14, Ma14, MY17, MAD12, MBKH19, MSG16, MZB+13, MFF11, MK10b, MK12, MLC+11, MCP10, MMR+10, MCC12, MV18, MP12, MTL+12, MSC10, MM19, MOY13, MMWA11, MNC+19, MUNVR12].

study [MUPC10, MDNDO+16, Men10, MFZ+18, MCL11, MGG13, MS17, MHP+17, MM11, MSK+12, M+11, MGD11, MTS15, MPRCEG12, MMRA10, MML+11a, MLA+12, MBBT12, Mor11, MM13, MG10, MMF+13, MSRn+11, MSOV13, MCAS16, MOH+12, ND11, NS10a, NHG+12, NDH10, NBL12, NAK+17, NTNL10, NL11, NFQ+11, NHBI2, NRG51, NRS+11, NRP+11, NRHJ11, NAJ+12, NT16, NZAVR10, NEE15, OAC17, OPI17, OAA19, OH12, OH13, OCB+10, OPP+14, OMD13a, OM13b, OD12, OD16, POLV12, PSI3a, PEA+12, P+11, PW+18, PDNC14, PMH+16, PE11, PWL+10, PSK19, PK13b, PKK14, PRG+10, PAD+10, PRP+13, PM17, Puz10, QS11, QCW+12, Qu13, RYM12, RNF+12, RGPD13, RRVJ10, RS12b, RSN12, RSM12, CRC+19, RD14, RRRV19, RGST12, RDB19, RYW+15, RI19, RCM10, RJLPGH+13, RDM+11, RBVAG18, RNE10, RNB+10].

study [RS11b, RRB12, SF13, SB18, SSB19, SIT+12, SK14, SD16b, SBEH11, SK11, SRYGV12, SB10a, SKHN13, Sat11b, Sch12a, SK17b, Ser11a, Ser11b, SLS+14, SKS11, SHT+13, SLSZ13, SHE10, Shi13, Shi18, SL10, SKM11, SM13, SR13, SSTD11, SLA12, SK11, SR18, SSA18, SSP+17b, SB18, SMA11, SZ11, SBB16, SZZZ11, SZZ+12, SLZH12, SHW+13, Sri18, SMGZ13, SK10, STU19, SYQ+10, SWS12, SWS+14, SZL+14, SZZ+15, SGL19, SYY16, SCZH16, SS13, TK16a, TV13, Tav11, Tav12, TM13, TT10, TDOID7, TU10, TLY10, TSL11, TFZ+15, TJ17, TFA10, TSH17, TFB11, TCCI10, TGA+11, Tug13, TWR15, TPT+13, TPT19, UKF+11, UMS13, VF13b, VPGC12, VFCSC17, Var11, VHTEG15, VNF+16, VLM+10, Ven12, VSMK13, VSMK15, VV12, VV13, Vie17, Vik13, VKF+19, VDG13, VS19, VO11].

study [VO12, WML10, WXZ+11, WJL+11, Wan11, WvRSW+11, WLL11,
QSX⁺15, RAN18, RNdA⁺10, SDS19, SDS20, SW10, Tou13, VLK⁺11, Xu16, Xu19, ZX12, ZWL18. **Systematic** [KSS12, WR15]. **Systems** [GLT13, IA13, KBF⁺13, ONK⁺13, ARG11, ACT19, Bae16, BR08, BR12a, BBB⁺12a, Brå11a, BDP12, BWE16, BBA⁺16, Cap16, CJBBMAPR19, CAPGAIG18, CH17, CS13, CP11, CP16, DMAB12, DLMRFY10, DBTA19, DCD10, DI18, Dun15, DB15, Fer19, Fin16b, FSST16, GB10, HS11a, HITU16, HFdGC14, HKLW13, IFT14, JE10, KH12, KK13, Kha16, KCC13, KSD10, KSN⁺10, KYH⁺13b, Kon11, Kry11b, Kry12b, KM19, Lad14, LS17, LV16, LGZC15, LC19, LRMAA19, SBD13c, WLL⁺13, XLLZ10, YGLL10, dOR10]. **Systems** [VOAH18, WCM14, XTLA13, XTLA14, YYI⁺12, YWH12a, YWH12b, Zak16, Zak16, ZWE12, dGR14, dOR10]. **systems** [Mam14]. **Szeged** [Tra19]. **T** [BL12, BTH18, CPF⁺11, SLS⁺11, ZHL⁺19, GWM11, BBM17, BTH18, SD13c, WLL⁺13, XLLZ10, YGLL10, dOR10]. **T-cell** [WLL⁺13]. **T-junction** [SD13c]. **T** [DFF⁺13]. **Table** [Gar08, GI10, Kut10]. **Tables** [Rus14]. **TACA** [Ser11a]. **Tailored** [GbZA10]. **Tailoring** [AV19, BHAH⁺18, MMA10]. **Take** [PUGSFM18]. **Tame** [DB13a]. **Tardy** [FK18]. **Target** [HM10b]. **Targets** [PUH⁺11]. **Tartaric** [LCZL11]. **Tautomer** [dAVdM17]. **Tautomeric** [SOM10, CCL⁺10, JN13, LDW⁺11, NRS⁺11, NJA⁺12, TSH17]. **Tautomerism** [HS11b, PS13a, VF13b]. **Tautomerization** [JS17, YY18b]. **Tautomerizations** [MPGS19]. **Tautomers** [KAOB11, LCH14, TAV11, TAV12, ZR13]. **Tayloring** [PJP08]. **TB** [ZCP11]. **tBu** [HHL12a, HHL14, PP14]. **Te** [ZLY⁺14]. **TCD** [WWX⁺11]. **TCNE** [TD11, KBMM10]. **TCNE-methylsubstituted** [KBMM10]. **TD** [AFC⁺10, BDR12, JPPA10, ACF⁺11, BVCAP12, FPQGMBI12, KI15, LJI13, Mas10, dSM19a]. **TD-DFT** [KI15, LGS⁺16, dSM19a]. **TDDFT** [WKE17, BGFD14, BAA⁺18, BHAH⁺18, ESDO16, HKLW13, IHG10, LY11, LZ10, MMWA11, PJP08, PSK⁺13, VSN⁺11, YZW⁺15a, ZSAP11]. **Te** [AM18, BHA19, WSML16, XWC11a]. **Tea** [MKHM11]. **Technical** [KdSM⁺10, LKJ13, MJSC18, SR12, SOF⁺10]. **Techniques** [DW12, LSR⁺10a, LSR⁺11, MQG13, OLS11b, RW11, SKV12]. **Technology** [YSA⁺11]. **Teller** [DMAB12, AGPDZ13, DMAB12, GFB12a, HR12, HFZ12, JZP17, RGPDZ13, SBD⁺16, TPCJ⁺12, WLZ18, YYI⁺13, ZFC12]. **Teller/Renner** [DMAB12]. **Telluride** [KG08, MW15]. **Tellurium** [ESDO16, RR19]. **Tellurium-containing** [RR19]. **Temozolomide** [KdPNS16, KMMS17]. **Temperature** [Buc12a, GFPVA19, KKH⁺13, MKSG13, PMMG⁺11, Boc12, CAAI12, CS17, DUN15, KAR12a, ILBQ⁺19, LL19, MOH⁺12, NAG17, TD11, WCGD12, AFV12]. **Temperature-dependent** [GFPVA19, ILBQ⁺19].
Temperature-programmed [ÁFV12].

[[Chu12, STM17].

tendencies [SMP10].

Tensor [SPM15, BL19, Fin14b, JMX15, LHX19, Lya14, NIT16, XXJ16, XWP18, YXM18].

Temperature-programmed [YFY17].

terephthalate [TNI13].

term [IIH16, Ols11b, ZLJ11].

terminal [SLS15].

terminated [dLDodAD12].

Terms [Gin10, Glu13, KLI11, PE11].

ternary [KYLC19, MS14b, OGvSG18].

tert [AMAC12, Pli18].

tertiary [MMM12, PCML08, SAG13].

test [DAA16, Mar12, PWP13].

Testing [FCS13b, KK14a, FCS13a].

testosterone [KKM12].

tetra [QJ13, SSA18].

tetraammine [MGK19].

tetraanions [DOZ12a].

tetrabenzozyophyrin [LGS16].

tetracarbide [PKK14].

tetracarbindane [ALK19].

tetracarbon [ALK19].

tetrachloride [YSA11, ZSZ14].

tetracoordinate [YD17].

tetrad [DKS11].

tetraad [DKS11, DKS11].

tetrafluoroborate [MFK12].

tetrafluoromethane [VVJ15].

tetrahedral [GAPK19a, IIV11, MPB10, Pup11a, RFFGPP16, TGA11, WQW17, YGL11].

tetrahedrofuran [dSDSPG11].

tetrakis [ZSASS13].

tetramer [FRNM12].

tetramers [MFOH18].

tetramethyltin [DAE12].

tetranitride [XXJ16].

tetranitrooctahydromidazoo [CC11a].

tetrahene [ZLS18].

tetrahene-bridged [ZLS18].

tetraphenybutadiene [VV18].

tetraphenylimidodiphosphinate [SLS14].

tetrapyrole [ZQJ10].

tetrasulfonate [DOZ12a].

tetrasulfur [XXJ16].

tetrazole [PP19b].

Tetrel [XCL18, WLC17, ZHL19].

TH [ZHL19, dOR10, JLI18, LNGW14, LLY19, NZL15].

Th-based [LYW19].

THDDP [SSKS12].

THDP [SSKS12].

Their [She14, ALK19, ALB18, AMI10, BPT12, Buc12b, BO11, BSO11, CJBMAMPR19, CCL16, CFV18, CTW12, DSC11, For12, GTR11, GWZ14a, GI10, HS11b, LLY19, MW19, MKM11, MMC19, PR10a, PL11, PSK19, RB10, RBZ15, RLR14, Rua10, SACA18, SM14c, VGGPD19, WJ11, XSL12, YZ11, ZR13, ZGS15, ZF15, ZYL13].

them [WXB11].

Theobroma [dAGNJ12].

theorem [GW13, Lev10, Nag10].

theorems [LB14b, Tch16, ZWE12].

theoretic [AB18, IOO18, YOS15].

Theoretical [AB18, IOO18, YOS15].

Theoretical [AB18, IOO18, YOS15].

Theorical [AB18, IOO18, YOS15].

Theorical [AB18, IOO18, YOS15].

Theorical [AB18, IOO18, YOS15].
[LDW+11, LXW+12, LWZ+14, LZZ+17, LLW+12, Lu10, LWC+10, LMCZ11, LCZL11, LCS+11a, LCH+11, LCS+11b, LXLL11, LW13, LYD+18, MLW10, MWH15, Mas10, MOY13, MDNDO+16, Men10, MAP+10, MMCNV19, MSK11, MJ14, MMV+19, MHHPR+17, MGD11, MBBT+12, Mor11, NYA+13, NL11, NMP14, NFD+10, NFQ+11, NH11, NHB12, NIT16, OT14, ONK+13, PEA+12, PWP+18, Pan16, PMEP19, PSKV19, PKK14, PMC11, RFN+12, RMLPGGH16, RI19, RCM10, Riv11, RGS+13, SK12a, SRASZ16, SLS+14, SLSZ13, SSA18, SZZZ11, SLZH12, SM14d, SK12b, SK10, SLS+15, SZL+15, SCZH16, TYN13, THWZ14, TM13, TYL10, TXL10, TSH17, TBF11, TGA+11, TPT+13, TPT19, UKF+11, VF13b, WXB+11, WLL11, WLG+11, WLZ+12b, WHS+13, WHY+14, WTW+15, WWQG17, WHM14, WZZL10, WLL19, WJ11, WSL+11, WWGW18, XGH18a, XZL+12, XWC11b, XbX+13, XCY15, XLZ+19, YZ13, YZL+10, YJ17, YHLC15, YC13].

Theoretical

[Zha10, ZZX10, ZLLS10, ZYZ+11, ZZR+12, ZSHL14, Zha14, ZQW+17, ZYSW17, ZSQ+10, ZFS+11, ZL12, ZSS+13, ZTC11, dSdSG11, dARAV12, dOdONM12, AZD+11, ASD14, AG19, BLL+13, BLB+18, BLRdA+10, BG13, yBZfC18, BPSM12, Buc10, CZH12, Cao17, CHH+19, CG12, CYLL11, Che12, CHL14, CZCW19, CGIA12, DP11, DDY12, DPK12, DTEMK11, DZ1a, DQZF12, DC12, EI11, EMED+12, ENV15, FMP+17, Fri12, GLF+12, GHGF12, GLXL18, GT13, GP13, HYZ13, HSS18, Iku17, Jia10, Jia15, KO14, Kim16, KC19b, KO12, LS17, Lan10, LR+11, LL11, LS19, LCZ15, LMC19, LLZ10, LX13, LW15, LdAA+11, MNP19, MCP10, MMR+10, MPR12, MLPT10, MUPC10, MEF+15, MEEA+13, MSRn+11, MSOV13, MMS19, ND11, NHC+12, NBL12, N´em14, NRS11, NRS+11, OKR12, OAA19, OH12, OH13, OMD13a, ORJ18, POLV12, PM17, Puz10, RGR12, SF13].

Theoretical/computational

[N´em14].

theoretically

[SA18, SFL+10, SSK11, SC12b, SKS11, SST11, SACA18, SRA+11, SYQ+10, Tch16, TK16b, VATPR11, VFSC17, VLM+10, VSMK13, VKF+19, VO11, WGLX10, Wan11, WLZ+12a, WZM+13, WWB+14, XF19, YM12, YZZH15, YLW+13, ZAE10, ZWY10, ZR13, ZKW17, ZPB12, ZW15, ZLWZ16, ZMB+17, dLR11, dOR10, doCMu1dALR11, DJB10, DC10, HHL14, LEU+11, Sit15].

theoretical/computational

[N´em14].

theoretically

[Jeo18, VMC11].

theories

[Cam10, JNZ+14, Li15, Luz08, ZT13].

Theory

[Ano13-49, BHA19, Buc12b, DCZ17, HKL13, ISN13, IKN13, Koc13b, Kri13, Kut13, LMZY15, MIN13, NS13, SSI+10, SSK+12, SIS+08, SKY+13, TKN13, TH13, YSS+10, YKN13, YH14b, AC19, ABM+19, AM13b, AGPDZ13, BVP13, BAX+19, BGBV12, BKBL11, BljdM12, Cam12, CCL+13, Car19, CFGMK12, Cha11, CH17, CM12, CZLD17, CC19, CK17, CF14, CTDOLA10, CSTA16, DWJZ11, DCCB11, DKS11, DLRMY10, DBl1, DMWY11, DGR+16, DG19, DCHC11, DSZB18, FZX18, Fin17, FA17, FMM1+10, Fri12, FSST16, GFPAV19, GCK+17, GM11, GEL18, GS11, GCZ+14, HMA+19, HR19, HLZ+14, HZZ+19, HM10a, HM10b, HI13, HYD11, HMA+18, IN15, IROW10, JR12, JPP+11, JHS18, JM+15, JW18, Kar12a, KCDC15, KC18, Kar13, KKL+16, KSAK17, Kit14, KM12c, KYLC19, KdSM+10, KJ14,
KMU\(^{+13}\), KFJ\(^{+18}\), KLE\(^{+19}\), Lar\(^{12}\), Lat\(^{13}\)]. **Theory**

[LPO\(^{+12}\), LCL\(^{+10b}\), LW\(^{11}\), LWL\(^{+12}\), LPG\(^{+12}\), LBY\(^{+14}\), LHX\(^{+19}\), LLW\(^{+11}\), Lin\(^{14}\), LDZG\(^{16}\), LLZ\(^{+12}\), Lya\(^{14}\), LKd\(^{+16}\), MYZ\(^{+10}\), MLW\(^{+14}\), MJ16a, Mam\(^{14}\), MLC\(^{+11}\), MFK\(^{+12}\), Mas\(^{14}\), MW\(^{16}\), MLK\(^{17}\), MLB\(^{+12}\), MBBT\(^{12}\), Mor\(^{13}\), MJM\(^{19}\), MCRS\(^{16}\), Mur\(^{12}\), Nag\(^{15}\), Nag\(^{17}\), NSN\(^{17}\), NS10b, Nak\(^{+17}\), NTLN\(^{10}\), NL11, NMIP\(^{14}\), OK\(^{16}\), OD\(^{16}\), PS10b, PS14, PK\(^{13a}\), PABSK\(^{16}\), PP\(^{16}\), Pat\(^{15}\), PTH\(^{11}\), PR\(^{10b}\), PBB\(^{15}\), PU\(^{14}\), PM\(^{16}\), PJ\(^{10}\), PMAP\(^{12}\), PI\(^{16}\), PC\(^{13}\), QBRA\(^{18}\), RGPZD\(^{13}\), RCM\(^{+19}\), RB\(^{18}\), RMG\(^{+19}\), RMC\(^{19}\), RAMB\(^{18}\), RS\(^{09}\), RS\(^{11a}\), Rud\(^{12}\), SVRGV\(^{12}\), SLC\(^{+18}\), SN\(^{15}\), SN\(^{12}\), Sha\(^{18}\), SZZ\(^{+10}\), SLZ\(^{+11c}\), SLS\(^{+11}\), SHL\(^{+13}\), SJZ\(^{+18}\), SM\(^{12}\), Stol\(^{18}\), SKZ\(^{12b}\), SD\(^{13c}\), SS\(^{13}\), TFBG\(^{14}\), TIN\(^{13}\), Tan\(^{13}\), TTD\(^{13}\), TH\(^{12}\), TDOD\(^{17}\), TG\(^{16}\), TXK\(^{19}\), TLC\(^{17}\), UV\(^{18a}\), VP\(^{12}\), Var\(^{11}\), VUC\(^{13}\), VBO\(^{+15}\), WKE\(^{17}\), WJL\(^{11}\), WW\(^{11}\), WJY\(^{15}\), WB\(^{17}\), WD\(^{+17}\), WTZ\(^{+11}\)].

**Theory** [Wit\(^{18}\), XNL\(^{+14}\), XGH\(^{+18b}\), YKM\(^{+15}\), YLH\(^{+19}\), YWH\(^{12a}\), YWH\(^{12b}\), ZS\(^{11}\), ZQCJ\(^{10}\), ZLW\(^{13}\), ZCX\(^{16}\), ZBG\(^{19}\), ZMZ\(^{13}\), ZSZ\(^{14}\), ZZ\(^{18}\), Zho\(^{18}\), dCSD\(^{dMC}\(^{13}\), dSTH\(^{17}\), BM\(^{10}\), SP\(^{19}\)]. **Theory-based** [KSAK\(^{17}\), WJY\(^{15}\)].

**Thermal** [GI\(^{11f}\), SMR\(^{14}\), TKSK\(^{17}\)].

**Thermalization** [Nes\(^{11}\)].

**Thermalized** [PFdM\(^{13}\)].

**Thermally** [GMM\(^{18}\)].

**Thermochemical** [Kim\(^{19}\), Rus\(^{14}\)].

**Thermochemistry** [ABTW\(^{14}\), S¸BAT\(^{16}\), AK\(^{11}\), BYAT\(^{13}\), ÇT\(^{14}\), HZG\(^{12}\), Rus\(^{14}\), WZX\(^{15b}\)].

**Thermodynamic** [JAB\(^{12}\), VOAH\(^{18}\), XNL\(^{+14}\), COCF\(^{+14}\), DWGX\(^{12}\), Kim\(^{13}\), LZZ\(^{+13}\), OSJ\(^{+12}\), Fan\(^{19}\), PP\(^{19a}\), RMLPGG\(^{16}\), Tav\(^{11}\), TSH\(^{17}\), dOLd\(^{1V}\)].

**Thermodynamical** [Nag\(^{17}\)].

**Thermodynamics** [MLW\(^{16}\), PK\(^{16}\), ByWG\(^{14}\), Bra\(^{19}\), DP\(^{11}\), PD\(^{11}\), PRFR\(^{17}\), RTG\(^{+19}\), WSCL\(^{11}\)].

**Thermoelectric** [KG\(^{17}\)].

**Thermostats** [GVPCK\(^{10}\)].

**These** [MMM\(^{19}\), Ril\(^{10}\)].

**Thiophene** [HHL\(^{12a}\), HHL\(^{14}\), AG\(^{10b}\), RTT\(^{10}\)].

**Thiazole** [MMB\(^{12}\)].

**Thiosemicarbazone** [LWH\(^{12}\)].

**Thiourea** [LCM\(^{11}\)].

**Third** [KWC\(^{11}\), MMF\(^{+13}\), NKF\(^{+13}\), RS\(^{09}\), RS\(^{11a}\), WLZ\(^{+12a}\)].

**Third-order** [MMF\(^{+13}\), NKF\(^{+13}\), WLZ\(^{+12a}\)].

**Third-row** [KWC\(^{11}\)].

**Thoughts** [KN\(^{15}\), Lev\(^{16}\)].

**Threading** [WMK\(^{+19}\)].

**Three**
[DMS$^{+10}$, FMMD$^{+10}$, HYH$^{+10}$, Kry10, LQZZ12, MPD$^{+15}$, MMP$^{+18b}$, RAN18, ARG11, Buc10, Buc11a, CG12, GsaY11, Hog13, KV19, LWY13, Mat02, Mat10, MUPC10, RZSZ18, RAGM10, SD13b, SYL$^{+18}$, SKY$^{+13}$, WvRSW$^{+11}$, WLZ$^{+12b}$, Zha14, JA12]. Three-body [RAN18, ARG11, Hog13, RAGM10]. three-center [Buc10, Buc11a]. three-dimensional [DMS$^{+10}$, MPD$^{+15}$, RZSZ18, SD13b]. three-electron [Buc11a, CG12, LWY13]. three-membered [Zha14]. Three-peak [HYH$^{+10}$]. three-photon [WLZ$^{+12b}$]. three-state [GsaY11]. three-unit [LQZZ12]. threonine [WJY15]. threshold [HMH$^{+13}$]. through-bridge [KyH13a, Na12, Na13]. through-space [CDT12, Na12, Na13]. throughput [CRFR11, KG17]. Thymine [TWHZ14, HYD11, TSH17, XSLF12, YM13]. Ti [FTB11, HLMO11, JL12a, KYLC19, MLY$^{+16}$, TFB11, ZLY$^{+14}$, CAZ$^{+11}$, NKWT19, OPP$^{+14}$]. TiCl [BAB$^{+18}$]. Tietz [KBG17, AAHN16, HRT12]. tight [BLB$^{+18}$, LNI12, WDJ$^{+17}$]. tight-binding [BLB$^{+18}$, LNI12, WDJ$^{+17}$]. Time [Bae14, BDF$^{+18}$, CP10, CW13b, HS11a, HKZZ15, HB14, ILBS10, SSAM13, Sko16, ZLE17, Bae16, BDF$^{+16}$, Brä13, CEFMK12, CW11, DZC17, DP11, FNIT16, HR13, HHCA10, IFT13, IFT14, JPP$^{+11}$, LMZY15, Luz13, MJM19, NNSN17, NNSN17, NDP10, Oht13, PV11, PV12, PJP10, PMAP12, PI16, RBGGM18, SL13, SHW$^{+13}$, SKV12, Vik11a, Vik11b, WKE17, Xu19, YLYC18, ZCG$^{+17}$, ZSZ14, ZZ18, Zho18, ZQCJ10]. Time-dependent [Bae14, BDF$^{+18}$, CP10, CW13b, HS11a, HKZZ15, ILBS10, Sko16, ZLE17, Bae16, BDF$^{+16}$, CP10, CEFMK12, CW11, DZC17, HHCA10, JPP$^{+11}$, LMZY15, Luz13, NDP10, Oht13, PV11, PV12, PJP10, PMAP12, PI16, SL13, SHW$^{+13}$, Vik11a, Vik11b, WKE17, YLYC18, ZCG$^{+17}$, ZSZ14, ZZ18, Zho18, ZQCJ10]. Time-independent [CP10, ILBS10, ZSZ14]. time-reversal [NSN17, NNSN17]. times [PR11a]. TiO [MFZ$^{+18}$, ATS15, ALA15, EFO11, EO11, GP13a, HCL13, OGvSG18, TFSRM11, XMZ$^{+12}$, ZK12, ZLWY13, ZDZL11]. TiSi [DHYC19]. TiSiO [MBKH19]. titania [SFNC$^{+18}$]. Titanium [YSA$^{+11}$, ALA15, Che13, DHYC19, OH13, RALK18, WWLZ17, YHL$^{+13}$, ZSAP11]. titanium-doped [DHYC19]. titancenyl [Con10]. Ti [LXD13, MIL10]. TM [PP19a, WSL$^{+11}$, YL11, BLDV19, WSL$^{+11}$, YL11]. TMZr [PP19a]. TO/H [ZHL$^{+19}$]. tolerance [Kan17]. tomentosin [ZRGE$^{+19}$]. tool [May14, MML11b, Sic16, TRZ$^{+19}$]. tools [VLG12]. topo [MBBT$^{+12}$]. topo-geometrical [MBBT$^{+12}$]. Topography [AS19, dOoCMuALR11]. Topography-driven [AS19]. Topological [MSAB19, AOT$^{+18}$, BL10, BLDV19, BCNR18, DM12, HYD11, JXX$^{+15}$, LNGW14, MZB$^{+13}$, MGB18, OAT$^{+13}$, PH12, PL11, PO15, TM19, BF11]. topologies [ART08, YWH$^{+12c}$]. Topology [AGNS14, BL10, FMKJ14, GRGRRHT19, Jen13]. tops [PBB15]. toroidal [CTDOLA10]. torquoselectivity [AMMB$^{+18}$, MB13, MBSMJ18]. torsion [DSCO$^{+13}$, GWME18]. torsional [CMCN11, MCMN$^{+11}$, RA10a]. Total
Transfer [SS10, AKC10, ARH+13, BSS16, CS17, DS11, DAA16, FV11, FDMR11, FSBA12, GI11a, GHCMMMMQ17, Jdl08, KyH13a, KUS19, KAOB11, KT12b, KBMM10, LZZ12, LYS+19, LYL+12, LXW+12, Lu10, MANP17, MPE15, MOGM18, MNC12, NMS+10, NBZG16, OK19, QJ13, RY12, RS12a, SS11, SMRK18, Sch15, SHS+13, SCS15, Tav11, Tav12, TCG13, WJ11, XDM+10, YH14b, Zen11, ZZ18, ZB18, dA12, dCDC+11]. 
transfer/induction [dCDC+11]. Transferability [GSR12, STM17, RLER10]. transferred [HSN18]. transfers [KyH13a, YYS15, YY18a]. transform [SFY12, YSO12]. transformation [DMAB12, DM12, DK13, HHC18, IM15, Jor15, Jor18, Man13, Rua10, SN15, TSS+15]. transformed [Hor13]. transistors [SAHA16]. Transition [BLdV19, Pie11, ALK18, BEM11, BZBZ13, Ber13a, BVP14, BB10, BDR12, Buc11a, BN11, CWW+16, Cho16, Cho19, CP13, Dau16, DMS+10, DMBL16, EMED+12, EMEPD15, GRLA18, GFB12b, GM11, GZBH18, JHL+18, KCW11, Kin13, Kry12c, Lar12, LCB10, LKd+16, MKM11, NKWT19, NZ13, Qu13, RZC13, SDS19, SDS20, SFW12, SAHG11, TMC+13, TT13, VSMK13, VO12, WWC17, WR15, ZK12, ZFC+17, ZHL17, ZS14, Zil14, KAR12a]. 
translational [Ld14, T11b, XTLA13, XTLA14]. translations [Hog10]. 
transmembrane [KMT+12]. Transmission [RBGGM18, CDT12, NTG18, NA12, SD13c]. transmitted [Cho15]. 
Transport [Yam11, DCZ17, DLZ11, ETGLMJ+19, Gao12, Jan10, JR19, KMI12c, MSG16, MMP11, OH12, OH13, PFdM13, RBGGM18, RRRV19, SS11, SSB12a, WDS19, ZY9+11, ZQJW13, ZY13, ZB18]. transporting [MCL11]. Trap [YZZ15]. trapped [TG13]. Trapping [PDNC14, LL18]. treatment [AEKGZ12, BHV+11, ISN13, Jor18, KL11, Kry12a, Man13, MSNP18, PMGMG12, SKG11, SSAM13, WJY15, AM13b]. trees [AD17, Bib13, DZ11b, Du12, LSW19, LWY19, LZZ19, PL18a]. trends [BCHN16, DMBJ15, MT10]. tri [AM18]. tri-coordinated [AM18]. 
triazol [CLY12], triazole [LLW+11, THSR13], triazol [IK14], tricarbon [ZJC+13], tricarbonyl [YZW+15a], trichelates [LOHB13], trichloroacetyl [SKS11], tricks [SCB+14], tricyclic [ZWK19], triagonal [HFF12], tridiagonalization [ZH12], triel [CDL+19], trifluoride [DGX12, For12, LQ13], trifluoroacetone [NRGS11], trifluoroethylene [OCB+10], trifluoromethylphenyl [SAHA16], trifluoromethyl [SKS11], tricks [SCB+14], tricyclic [ZWZK19], tridiagonal [HFZ12], tridiagonalization [ZHF12], triel [CDL+19], trifluoroacetylacetone [NRGS11], trifluoroethylene [OCB+10], trifluoromethylphenyl [SAHA16].
SOF$^{+10}$, SN12, SSAM13, SZS$^{+10}$, SLZ$^{+11c}$, SLZ$^{+11a}$, SLS$^{+11}$, SB10b, SM12, Sri18, SK12b, TNN16, TMC18, TG13, TWR15, Val17, WML10, WB17, WDJ$^{+17}$, WH12, XTLA13, XTLA14, Xu19, ZWSF16, ZS12. using [ZZ18, ZCP11, dAB17]. utoferin [KSY$^{+11}$]. utilizing [KFS13, Tou11a].

UV [AFC$^{+10}$, BSS15, Bou12b, ÇAS13, DSD18, FPRGMHGB12, MSBF18, PJP08, PJP10]. UV-Vis [DSD18]. UV-visible [Bou12b]. UV/VIS [PJP10, PJP08]. uvarovite [MPZWD10, VPFD10].


Valence [Lu10, Tch13, TFB11, ZLY$^{+14}$, Ang10, AMK10, BN11, KWC10, ILBqD$^{+19}$, LW18, NKWT19, NTNL10, SS13, TD11, XCL$^{+18}$]. V-shaped [BN11]. VA [Eng16].

vapor [Chu12, LKOS17, TFBG14]. variants [RPBB11]. variation [JWG$^{+12}$]. Variational [FAFR12, CDS$^{+18}$, DSSM18, Kri13, NS10b, Oht13, dMOB12, SBM16, SSB12a, Shai1a, ZSI1, MHT$^{+08}$]. variations [KBGC12, MB12]. variety [AM10, TOSN12]. Various [MGK$^{+12}$, ART08, HFL$^{+17}$, KMT$^{+12}$, PSK$^{+13}$, SMM11, STM13, YÇÖ11].

vapor [Chu12, LKOS17, TFBG14]. variants [RPBB11]. variation [JWG$^{+12}$]. Variational [FAFR12, CDS$^{+18}$, DSSM18, Kri13, NS10b, Oht13, dMOB12, SBM16, SSB12a, Shai1a, ZSI1, MHT$^{+08}$]. variations [KBGC12, MB12]. variety [AM10, TOSN12]. Various [MGK$^{+12}$, ART08, HFL$^{+17}$, KMT$^{+12}$, PSK$^{+13}$, SMM11, STM13, YÇÖ11].

Viable [fXxBhD19]. vibration [HK11, HRT12, KBG17, LZW$^{+15}$, QD10, SPO$^{+11}$]. vibration-rotational [SPO$^{+11}$]. Vibrational [AC12, CTVA12, Cyb11, FKL$^{+12}$, KKT13, KKT14, SD12, AF19a, AGCVG15, BBB$^{+12a}$, BBB16, CP10, DK13, DCFD10, DWGX12, For12, FKC12, dDG110, HH18, Ish14, KL11, LWJ$^{+11}$,
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LWWZ13, MC11a, MBKH19, MCE11, MB14, MMCN+ 11, NDM+ 12, PM12,
PBB15, RPBB11, RSM12, RC11, Roy14, ŞBAT16, SA11a, SPO+ 11, SZZZ11,
SZL+ 14, TU10, Tou11a, WHY+ 14, YWH+ 12c, ZGSM15, ZPZ15, ZQXP17].
vibrationally [LMZY15]. vibrations
[CNBPR+ 11, CMCN11, Eil14, LBW11, NH18, ZZ15]. Vibrio [PI13].
vibronic [PETB18]. view [AY15, BMRM19, BLdV19, vL13]. viewpoint
[LS19]. Vignale [PS13b]. VII [SIS+ 08]. vinyl
[BSSS19, DP12, KI15, WZZL10]. vinylallenes [LW11]. vinylation
vinylcyclopentadiene [VV18]. vinylidene [OCB+ 10]. vinylideneflouride
[OCB+ 10]. vinylideneflouride-trifluoroethylene [OCB+ 10].
vinylpyranoanthocyanin [COdF+ 11]. vinylpyranoanthocyanin-phenol
[KN15, CCA+ 12, CRFR11, KPH+ 12, LG10, Lya19, MSNP18, RMG+ 19,
SDP+ 16, ST15]. virtue [FYhC11]. viruses [WZ10a]. VIS
[PJP10, AFC+ 10, ÇAS13, DSD18, MSBF18, PJP08]. Visible
[FPRGMHGB12, Bou12b, WCL+ 17, dARAV12]. visual [LLLT12].
Visualization [Val13, Ash18]. visualizes [ABM+ 19]. Vitae
[Ano11a, Ano11c, KK12b]. vitamin [WTH+ 11, WLD+ 10]. vitro [CG12].
VIVO [MG12]. Vleck [Jør15, Jør18]. VMD [CRFR11]. VO [Che12].
Volterra [CYK17]. Volume [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e,
Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n,
Ano13k, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w,
Ano13a, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i,
Ano13j, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13x, Ano13-35,
Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31,
Ano13-32, Ano13-33, Ano13-34, Ano13-36, Ano13-37, Ano13-38, Ano13-39,
Ano13-40, Ano13-48, Ano14a, Ano14b, Ano14n, Ano14t, Ano14u, Ano14v,
Ano14w, Ano14x, Ano14y, Ano14z, Ano14c, Ano14d, Ano14e, Ano14f,
Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14o].
Volume [Ano14p, Ano14q, Ano14r, Ano14s, Ano14-27, Ano14-37, Ano14-43,
Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-48, Ano14-28, Ano14-29,
Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14-35, Ano14-36,
Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano15a, Ano15b,
Ano15c, Ano15d, Ano15e, Ano15t, Ano15x, Ano15y, Ano15z, Ano15-27,
Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n,
Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15u, Ano15v, Ano15w,
Ano16a, Ano16s, Ano16t, Ano16n, Ano16u, Ano16v, Ano16w, Ano16x,
Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16b, Ano16c, Ano16d, Ano16e,
Ano16f, Ano16g, Ano16h, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m].
Volume
[Ano16o, Ano16p, Ano16q, Ano16r, Ano17a, Ano17b, Ano17m, Ano17n,


**Volume** [Ano19r, Ano19s, Ano12o]. vortex [GKS10]. vorticity [BL19, HMH10a]. vs [Ali19b, DG19, SP19, Yam10]. VSc [BBYZ18]. V [LW18]. vsLab [CRFR11].

W [HNBS18, MLY+16, ZLY+14, GAPK+19b, SXS+12]. **W1BD** [VF13a].

W2 [OK16]. W2w [OKR12]. **Waals** [BPG+10, BAP12, Ber13b, GRCATG19, KKL+16, NRI15, PABSK16, SZZ+19].

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

Wannier [PABSK16]. warm [DW12, Ng12]. Watch [ZLWY13]. Water [Kim18, RFEGPP+16, WW11, XMZ+12, AF16, ATS15, BBB+12h, BPSM12, BCS+12, Cha10, CNSK11, Chui2, CK17, CAPL12, DPK18, DE18, EFO11, EO11, FMC11, FUE+12, GZS10, GLPA10, HDQ+13, HS11b, KK11c, KV11, LLF+12, LLM13, LJW+11, LNGW14, LCB10, Ma14, MAD12, MFB11, MK10a, MK10b, MPE15, Mar12, MTL+12, MPV+11, MOE+11, MD11, MRA11, NS10a, OHDA13, OD12, PW10, PCMG12, QSLY10, RRWJ10, RAK10, SYK+12, SSK+12, SMEH15, SMEH16, SK12a, SJZ+18, SL10, SCL19, SW12, SJW13, SML11, TGRP19, Var14, WCGD12, WWD+15, WTP+19, WSV10, X18, XGH18a, YY18a, YYY+12, YT14, ZKZW17, Zak13].


**Wave** [AB16a, HDOS12, Kut13, NS13, TKN13, TH13, YKN13, Bae16, BR12h, CW13b, Cho19, CSMZ10, D’y16, GBS17, Gao11, GKT+12, HR12, Hog13, IK18, KRC+16, KH10, Kar13, NGTC19, Oht13, OHDA13, OH19, RZ17, RW11, SSAM13, SGL10, Tobi19, WC14, WH12, YLYC18, ZHF12, ZCG+17].

Wave-function-based [AB16a]. wave-functions [Hog13]. wave-packet [Bae16]. wavefunction [CH17, DACK11, GWHH17, ZWSF16].

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

Wavelet [SFX12, GSPR19]. wavepacket [GWZ+14a, Hkzz15, Han19].

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PAKA15, VO12, XZZ\textsuperscript{+}10, XWC11a, YL11, Bal16, CRB\textsuperscript{+}12, DSD18, MC17, MRT11, ZSASS13, dCDC\textsuperscript{+}11. ZnO [ESDO16, BRBRS11, KA13, LPO\textsuperscript{+}12, MTL\textsuperscript{+}12, RZC13]. ZnO-based [LPO\textsuperscript{+}12]. ZO [EAV16]. zone [BG11a]. Zr [Bou11, Kim19, WJL\textsuperscript{+}11]. ZrF [BLKB11]. ZrN [RMLPGGH16]. ZSM [JLL11, SZ11]. ZSM-5 [JLL11, SZ11]. zündel [MNC12]. zwitterionic [KRG\textsuperscript{+}13, RFMC19, YZZ15, ZZ18].

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