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Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA
Tel: +1 801 581 5254
FAX: +1 801 581 4148
E-mail: beebe@math.utah.edu, beebe@acm.org, beebe@computer.org (Internet)
WWW URL: http://www.math.utah.edu/~beebe/

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Title word cross-reference

\((N - 1)\) [ACD\(^+13\)a, ACD\(^+13\)b]. \((n = 2, 3, 4)\) [VSP\(^19\)]. \((\sigma^3, \lambda^3)\) [TR\(^12\)].
\((\sigma^3, \lambda^5)\) [TR\(^12\)] + [CXW14, GTK10, NMLD13]. 0 [UD\(^12\)].

\([MG15, TS15b, YZLZ18]. 1 - n\) [CYG\(^+15\)]. 10 [AC\(^11\)b, TS\(^15\)b]. 13
[MYGW12, SIT18]. 15 [AC\(^11\)b]. 17 [GZZ\(^12\)]. 18 [LW\(^16\)]. 2 [CWT\(^+12\),
CBDS\(^19\), GSS\(^13\), MSBF\(^16\), MH\(^10\), SJD\(^14\), WvRSM\(^14\), YDL\(^+10\), YZLZ\(^18\)]. 20
[AC\(^11\)b, LYL\(^16\), YVEI\(^+17\)]. 24 [TS\(^15\)b]. 3
[AARP\(^17\), CM\(^16\), DVVP\(^14\), GMMH\(^+16\), GSS\(^13\), GPK\(^12\), GBG\(^+19\), HSW\(^+19\),
LT\(^16\), MG\(^15\), MA\(^16\), MYT\(^+14\), MP\(^19\)b, MSSP\(^17\), PSS\(^14\), Pop\(^18\), RVCFF\(^13\),
TS\(^15\)b, VVMY\(^18\), YLL\(^11\), YZLZ\(^18\), dL\(^v\)NC\(^18\)b]. 4
[AFSW16, GWJJ\(^12\), ZTH\(^+15\)]. 4d [Hil\(^13\)]. 4f [Hua\(^16\)]. 4 \times 1 [LGKS\(^17\)]. 4 \times 4
[SH\(^14\)]. 5 [APY\(^+16\), LZH\(^16\), WFL\(^+19\), YLL\(^11\)]. 5\(^+12\) [MKH\(^15\)]. 6
[MCAY\(^15\), Rab\(^12\), TSZQ\(^12\)]. 6\(^2\) [MKH\(^15\)]. 6\(^3\) [MKH\(^15\)]. 6\(^4\) [MKH\(^15\)]. 7 \times 7
[UGK\(^18\)]. 8 [CSC\(^+18\), TN\(^12\)]. 8 \times 2 [LGKS\(^17\)]. [2 + 2] [LXFC\(^17\)]. [5 + 1]
\[ \text{[CAT}^\pm, \text{JXSW}15, \text{MCK}17a, \text{TDKT}10]. \] \( f^n \) [\text{BBG}^\pm18b]. \)

\( \gamma \) [\text{BTB}^\pm11, \text{DBG}11, \text{YLCX}10]. \( J \) [\text{KNP}^\pm12, \text{LZH}^\pm11]. \( k \) [\text{Hug}14, \text{YS}15]. \( \kappa \) [\text{YRSS}10]. \( \lambda \) [\text{BH}15]. \( \lambda^3 \) [\text{SLT}14]. \( \lambda^N \) [\text{XHLH}16]. \( \leftrightarrow \) [\text{RSK}^\pm15]. \( M \)

\[ \text{[ATIP}18, \text{AM}19a, \text{LLX}^\pm19, \text{MP}19b, \text{YLT}^\pm19, \text{NH}19]. \] \( n = 1, 2 \) [\text{SIT}18].

\[ m = 2 \) [\text{TS}15b]. \( m = 2, 3 \) [\text{TS}15b]. \( M_\gamma \) [\text{ATIP}18]. \( \mu \) [\text{RHPWS}13]. \( N \)

\[ \text{[AARP}17, \text{HPT}17, \text{JSW}10, \text{KYCL}11, \text{KYKR}15, \text{KSK}11, \text{LHL}^\pm10, \text{LXZ}^\pm10, \text{MB}16, \text{PHT}17, \text{PM}18b, \text{QZM}11, \text{RF}15, \text{YLZ}^\pm10, \text{ZYW}^\pm10a, \text{ZBP}11, \text{dSdLBN}17, \text{BLBG}^\pm13, \text{BS}10b, \text{HCB}11, \text{JLH}^\pm14, \text{LLX}^\pm19, \text{LXFC}17, \text{OKY}18, \text{RFF}11, \text{SLY}^\pm19, \text{TCGN}18, \text{TT}18]. \] \( n + m = 4 \) [\text{XhD}15]. \( n + m \leq 3 \) [\text{GT}10]. \( n = 0 \) [\text{MCAY}15]. \( n = 1 \)

\[ \text{[GWJJ}12, \text{Rab}12, \text{RVCFF}13, \text{TN}12, \text{TSZQ}12, \text{YLL}11, \text{TS}15b]. \ n = 1, 2 \ [\text{ABB}^\pm12, \text{ABB}^\pm13]. \ n = 10 \) [\text{TS}15b]. \( n = 12 \) [\text{YVEI}^\pm17]. \( n = 2 \)

\[ \text{[WYGW}12, \text{TS}15b]. \ n = 3 \) [\text{SIT}18]. \( n = 4 \) [\text{GZZ}12, \text{TS}15b]. \( n = 5 \) [\text{AC}11b]. \( n \leq 20 \) [\text{ASS}10]. \( n \leq 25 \) [\text{Tak}11]. \( n \leq 55 \) [\text{Tak}10]. \( N \log N \) [\text{AO}10]. \( O(N) \)

\[ \text{[BLS}11]. \ O(\log N) \) [\text{FGM}11]. \( p \) [\text{HN}17, \text{MCK}17b]. \( \pi \)

\[ \text{[AH}10, \text{BLBG}^\pm13, \text{BS}18, \text{CLFR}18, \text{CKL}^\pm11, \text{DLMH}12, \text{GNC}^\pm18, \text{GZM}16, \text{HSZ}^\pm11, \text{KV}14, \text{KDS}17, \text{MUN}^\pm19, \text{MVK}10, \text{MIS}^\pm15, \text{OOK}11, \text{PM}18a, \text{RF}15, \text{SSGS}15, \text{SDF}12, \text{SWW}^\pm19, \text{YJN}^\pm11, \text{Zha}11, \text{ZZW}19]. \pi \cdots \)

\[ \text{[YZZ}^\pm17]. \pi \cdots \pi \) [\text{CCCLCG}14]. \( pK_a \) [\text{BA}11, \text{CPK}19]. \( \Psi \) [\text{Lüc}14].

\[ q = 0, \pm 1, -2 \) [\text{XhD}15]. \( r^2 \) [\text{RMC}^\pm13b]. \rightarrow \)

\[ \text{[CK}10, \text{Chu}10, \text{GTK}10, \text{H}211, \text{HBL}12, \text{LWD}13, \text{NMLD}13]. \( \sigma \) [\text{KKL}^\pm13]. \sigma \)

\[ \text{[DPSL}16, \text{GZM}16, \text{LZL}^\pm15b, \text{PM}18a]. \sigma \pi \) [\text{CZY}11, \text{YWZ}14]. \( \Lambda \) \( \Lambda' \)

\[ \text{[MCLD}10]. \times \) [\text{SRS}14]. \rightarrow \) [\text{CSNCS}^\pm18, \text{SB}19, \text{XCLZ}19]. \( v = 0 \) [\text{LWD}13]. \( X \)

\[ \text{[AM}19a, \text{Sak}18, \text{UT}15]. \ x = 1 \) [\text{CWT}^\pm12, \text{LZTV}10]. \( Y \) [\text{UT}15].

-1 [\text{dLxNC}18a]. -5 [\text{LL}10c]. -A [\text{YJN}^\pm11]. -acceptor \) [\text{MIS}^\pm15]. -Ace \)

[\text{LHL}^\pm10]. -acetals \) [\text{YZL}^\pm15]. -Acetate \) [\text{BHP}19]. -Aceto- \) [\text{SJD}14].

-acyetyl- \) [\text{ZBP}11]. -acytation \) [\text{LHL}^\pm10]. -adrenergic \) [\text{LLHM}16, \text{VKC}10].

-\text{Al} \) [\text{YR}13]. -alkenoyl \) [\text{YZL}^\pm15]. -alumina \) [\text{SH}14]. -amination \) [\text{YZ}17].

-amin \) [\text{ZKH}^\pm10]. -aminopolyacrylate \) [\text{CMD}13]. -arene \) [\text{ZCK}^\pm16].

-atomic \) [\text{JXSW}15]. -ATPase \) [\text{II}10]. -azacrown-5 \) [\text{ZYW}^\pm10a]. -barrel \)

[\text{yOAC}10, \text{WXL}^\pm12]. -based \)

[\text{BPE}16, \text{EBK}13, \text{EP}15, \text{EB}18, \text{LFB}14, \text{MP}19a, \text{PBE}16]. -benzaldehyde \)

[\text{Lu}11]. -bipyridinyl \) [\text{KPL}15]. -block \) [\text{CAT}^\pm13, \text{MCK}17b, \text{TDKT}10]. -bond \)

[\text{CKL}^\pm11]. -bound \) [\text{XWSW}13]. -butane \) [\text{TCGN}18]. -butanol \) [\text{BS}10b].

-butene \) [\text{MSBF}16, \text{WvRSM}14]. -butyl- \) [\text{MG}15]. -butylbenzene \) [\text{HCB}11].

-carboxylates \) [\text{AARP}17]. -carrabiose \) [\text{YRSS}10]. -catalyst \) [\text{SSD}19].

-catalyzed \) [\text{YXZZ}17]. -cation \) [\text{MUN}^\pm19].

-chlorodiphenylacetohydroxamate \) [\text{CBDS}19]. -conjugated \) [\text{BLBG}^\pm13].

-coumaric \) [\text{HN}17]. -couplings \) [\text{LZH}^\pm11]. -Cu \) [\text{NGAS}17]. -curcumin \)

[\text{AKM}11]. -cyclodextrin \) [\text{DBG}11]. -dimensional \) [\text{MB}16].

-dimethylaminophenyl \) [\text{YLZ}^\pm10]. -effect \) [\text{RWR}^\pm13]. -electron \)

[\text{KTK}17, \text{LW}16, \text{LYL}16, \text{HPT}17, \text{PHT}17]. -erythrose \) [\text{SM}17]. -expanded \)

[\text{MLQ}^\pm12]. -F12a \) [\text{MLCD}11]. -form \) [\text{GWX}^\pm12]. -glucosamine
[LJW+11b, TKCN19]. -hairpin [LJW+11b]. -helices
[KKK+19, HHT+13a, HHT+13b]. -helix [CCOH14, WXL+12]. -heptane
[RSSF11]. -heterocyclic [KYKR15, LZX+10, RF15, dSdLBWB17]. -hole
[BSF18, GZM16, LZR+15b]. -holes [PM18a]. -hydrogen [GNC+18].
-hydrogenase [GS11]. -hydroxydimethylnitrosamine [FFA14].
-hydroxybutyrate [SJD14]. -hydroxymethylfurfural [APY+16, WFL+19].
-hydroxyquinolin-imidazolinone-based [CSC+18]. -hydroxysteroid
[BH15]. -LiCl [LCL+18]. -like [WGN+16]. -maltose [SWM10]. -metalloid
[MMS16]. -methyl [LZL+16]. -methyl-Imidazolium [MG15].
[NDG14]. -methylformamides [JSW10]. -Montmorillonite
[BHB19, BHB+17]. -N-benzyl-N- [NDG14]. -napthalene [CYY+17].
-nearest [Hug14, YS15]. -nitroaniline [ZTH+15]. -nucleophile [ZYR+15],
one [YZLZ18]. -ones [YZ15b]. -orbitals [MCK17a]. -organic [AH10]. -oxo
[VBMA13, RHPWS13]. -oxoalkyl-substituted [AARP17]. -Pd
dSdLBWB17. -pentane [TCGNT18]. -peptide [LLvG10, LvG13a].
-peptides [LvG13c, ZKH+10]. -phosphoranes [TR12]. -pinene
-propionic [CM16]. -pyridone [AFSW16]. -representability [PM18b].
salen [DSHLM18]. -secretase [YLCX10]. -sextet [KDS17]. -sheet
[CCOH14, WS10]. -substituted [LZH+16]. -system [SWW+19].
-thiaphosphiranes [TR12]. -turn [SZB19]. -type [SLY+19]. -types
[Pon10].

[DSHLM18]. /Fe [DAdGR15]. /GIAO [OPR16]. /GIAO-CCSD [OPR16].
/H [WLF19]. /metal [BSF18]. /MgO [BS16b]. /MM [CZY11]. /PDIxCN
[ZZL19]. /TD [TS15b]. /X [BSF18]. /Zn [GEP+14].

0 [KKH19].

1 [ZZWX11, CS17, DLZ15, GTK10, NH16, SYH12, SRS14, TTB+10,
UNT16, XLY12, ZAs10]. 1*- [ZZWX11]. 1-14 [GNI18]. 1-16 [XWSW13].
1-21 [GNI18]. 1-Methyluracil [HvM17, HvM16]. 1-Octene
[MJLV14a]. 1-penten-5-y1 [LXFC17]. 1.0 [SWB+12]. 1.1 [KJM+17]. 1.3 [LSL+19].
10-Phenanthroline-5 [SCSM19]. 10.1002/jcc.25747 [MT20]. 102
[RvdMB16]. 17 [KSM17]. 195 [PDGb+16]. 1D [AWF+18]. 1D-charge
[AWF+18]. 1H [YZ15b]. 1T [RSK+15].


7 [ADF+10, CD19, MBR+15]. 7-azaindole [YYT12]. 7-diphenylamino-9
8 [AAC+16]. 8-formyl-7-hydroxycoumarin [LZHH11].
8-naphthoquinone [HWB19]. 8R [BG13].


ability [LLL+10, PGS+15, RTS+13]. above [MK17]. Absolute [Gri13, HLW+17, KB11b, KYB13, VED10]. absorbing [NPG+18].
Absorption [RS17a, ZLL+10, DMD+18, FD13, HNN+17, KB16, LLBO12, LX11, LXZ+10, MKK+19, PMC+17, PDZT10, PDG+16, SGDT10, TYN15, TZ12, Tsi14, WWD14, ZTH+15, ZDX11, QCR12]. abstraction [AAMD+11, BS10b, CSXZ17, CY12, JCG+10, LJW+11b, PNE18, WLHZ12, dCRN18]. Ac [SNKS10]. ACCDB [MP19c]. Accelerated
[MFEM15, MFEM16, SH19a, YKNN19, AGB13, BDTP11, CVT+11, CF18, DWC17, GBL+11, HEMCZE+14, HAP+12, KV13, LL11, MLN+18, REU+17, YLX14, YSG12, ZC14, ZLL+13]. accelerates [HS17b]. Accelerating [HASR+12, HB19, LZ12, WYJ+16, HP10a]. Acceleration [BK+11, ON14, SOM+13, UTM11, WSGN11, OOT15]. accelerator [SBV10]. accelerators [KK17a]. acceptance
[BB11b, KB11c, NDW15, dBRO13]. acceptor [EHT19, Gil11, Lu11, MSV16, MB+15, SB19, ZSTR+18, ZLL19]. acceptor-bridge-donor [ZSTR+18]. acceptors [KKK+19, uH11, TZ12]. accessibility [HPL+18, LHL+10]. accessible [FZ+12, WXL+12, WBF17].
Accessing [JZZM14], accompanying [HSN14]. according [GM17, LPE+10, YZZ16]. account [EPH+13, Tsi18]. Accounting [XML+15, HH11, MBC11]. Accuracy
[ASW19, DBM+15, FCE15, KFY+13, LL17, BPB11, GRAR+14, HWL11, KSR+16, LZ12, LDZW17, MLG18, NTNY15, yOAOG10, RS13, RVCFF13, Rob13, TO10, VV+18, ZYS+10, AIM+18, Gil11, SDP+18]. Accurate [BS10b, BS18, CX10, CSXZ17, EFOD13, FL11, IN13, KG15, LYG+13, LL11, LWL+10, MK13b, MFR+11, NW17, Pol13, PVJ10, Sch12, SRR16, SY11, SSB+16, SYZ+17, TH13, VSP19, WL14, YB16, ZW11, ZLX11, ZYL12, ZLZ+19].
Algorithmic \[LPS12\]. Algorihms \[BV14, KGHC15, AGR11a, AC12, CD13, Fon11, GBSE11, KJM+17, Leh15, LLZA12, MS16, MO15, NC14, NOKJ16, RFN15, TRA+16, ZVY+15, dACP12, vLBBR12\]. aligned \[KC14\].

alignment \[BF15, HRK+10, HKRSL11, HS11, MJM+15, RP15, RHJ11, Ran12\]. alignments \[CYI+10, Ran13\]. aliphatic \[CROB16, SB10\]. Alkali \[YHCS11, Ano11, AM19a, DDM+15, JHMB+09, JHMB+11, THP+15, ZWY+10a\].

alkali-metal \[ZWY+10a\]. alkalides \[WXS+12\]. Alkaline \[XZ11, Ano11, JHMB+09, JHMB+11, WD10\]. alkaline-earth \[WD10\].

alkane \[JGS+17, ZST14\]. alkanes \[Jor17\]. Alkanethiol \[SJS19\]. AlkB \[PHC13\]. alkenes \[Jor17\]. alkenoic \[YFL+15\]. alkoxy \[WFL+19\].

alkoxy-catalyzed \[WFL+19\]. alkyl \[Den12, RMGB11\]. alkylthiols \[FVP14\]. alkyne \[WWTL19\]. alkynes \[Jor17, YYZZ17\]. All-atom \[SM14b, CS14, DPNM11, HM13, JYC+16, KT18, LZZ14, MZZ11, OCW+15, VHA+10\]. all-atomistic \[FPH+19\]. All-electron \[KKA+18, PGDo+16\].

all-organic \[LZL+15a\]. all-siliceous \[Lar11\]. allene \[GRCL12\]. allenes \[KV15b\]. allocation \[NOKJ16\]. allopolyacrylan \[RML+15\]. allostere \[DBK17, ILKR11, MWM+11, SR17, ZDT18\]. Allotropes \[OSI+19\].

allotropic \[GBK+19\]. allowing \[MLC13\]. alloy \[NIIT15\]. alloys \[GD10, vADC+14\]. ALMOST \[FSC+14\]. AlN \[wZbZ11\]. AIO \[GWPJ11\].

along \[ABDGN12, AC11b, CM13a, CX10\]. Alpha \[MH10, MBK+13, SPZP18b, XTY+14\]. alphabets \[PHDH13\]. A IPO \[LL10c\]. alter \[CBTZ16\]. alterations \[HHT+13a, HHT+13b\]. alternate \[ZWS+10\]. alternative \[ASL+11\].

alternative \[DSHLM18, MA17, NYN17, TF15, Wei12a\]. alumina \[SH14\]. Aluminum \[Kop19a, SBG18, WFL+19, GWJ12, LK16a\]. always \[KSC16, MBFG15\]. AM \[FBY+17\]. AM05 \[MMJ10\]. AM1 \[KLS10, KMLS0\]. AMBER \[MSK+12, RSR+12, MLN+18, GCW14, MSK+10, MGJ+15, OYK+11, PGW+17, SOY12, SJ16\]. AMBER-compatible \[SOY12\]. AmberTools \[RNSF+16\]. Ambident \[WBKS19\]. amide \[LJW11a, LW11, NDG14\].

amidoborane \[PMT16\]. amidoboranes \[DLT17\]. amination \[YZ17\]. amine \[AK10, BMB13\]. amines \[MR+18\]. amino \[BSG+18b, CCLGRO14, CFIC15, CB1d, DKET+17, FZL+15, FP17b, GRL+11, GRL+12, HCP15, KLS10, KMLS10, LXL+11, LP11b, MRO17, PHDH13, RSL16, SISK10, SBM13, SST+18, WC14, ZZWT12, ZKH+10, ZHXX11\].

amino-acid \[KLS10, KMLS10\]. aminoacid \[MC10\]. aminophenyl \[LZL+16\]. aminophthalimide \[WHL+10\]. aminopolycarboxylate \[CMD13\]. aminotriethylene \[MSY19\]. amrine \[dCCGRN19\]. ammonia \[BEMP14, CC12a, KT12, SNS16, SJZ+15, VS14\]. ammonium \[AvKSP16, DSHLM18\]. AMOBA \[HLW+17, MBE16, PZCL16, XP13\]. among \[KYB13, SH15, TCGNT18, WGL+11\]. amorphous \[Fom13\]. amounts \[FN12\]. amplitudes \[Les19\]. Amsterdam \[FPV13, SFG+17\]. amyloid
[IO13b, LH11]. amyloid- [IO13b]. amyloid-beta [LH11]. analog [JBAM11]. analogs [DCHL12, LP11b, SISK10, VM11, WBT10]. analogue [PGW +17]. analogues [LPS +13, NK19, SGWA17, VVBL17, VM19, WS12, YLL11]. analyses [BSF18, CBDS19, KASH14, KP11, PZBA13, SKGB13, VVJ15, XWW +11]. Analysis [BMD19, CDG +15, ELKE19, HAI +16, JCGM18, KKGW19, LL19a, MOS12, SZL19, SvLK18, Spr18, XFG +16, AKMT11, AST +16, ASL +11, ARRC15, AAB +19, AS18, ANO15-58, AM19a, AM19b, BK15, BL19, BH14, BSSP +13, BBG +18b, CMM18, CAL +13, CEBO15, CCH +11, CHT +13, CHY4, DMJ17, DDP +18, DTF +11, DJD12, DBK17, DJS +18, DCS15, DN19, ESD18, EHSP16, EB18, Fer17, FB12, FHW +11, FHK +12, GVP +10, GLW13a, GLW13b, GD +12, dCGCRN19, GCP +13, Han11, HSB +19, HCT +10, HPSK12, HHT +13a, HHT +13b, HGW18, HDHL15a, HDHL15b, HHWL17, Hug12, IY18, Jan16, JHH +13, JJW +14, JZZM14, JCX10, JLS18, KG13, KYG +15, LSL +19, LBC +19, LL13a, LCPS13, LMZ +11b, LFM12, LAHS16, LGKS17, MLG18, MDTD13, MJ14, MT19b, Mez10, MADWB11, MCLD10, MGS +16, MCK17b, NK19, NH19]. analysis [NIIT15, NS17, OXBW16, OC14, PTK11, PSP15, PRYI +17, PTB +15, PPUBGD10, PS12, PS14, RDT14, RSG18, RC18, REL17, RLG14, SFM +18, SLY +10, SBB10, SFR +11, SHFJ18, SSGS15, SEJ +18, SB18, SNDK16, SS13c, SB19, SPR +13, SH18b, SSP +19b, SH19b, TYN15, TCB16, TD10, TT +10, TS10b, UKS11, VBMA13, WNP +16, WWW19, Wei12a, Wei12b, WDKT19, XFG +15, YK13, YNH +17, Yes12, Yes15, ZCS +15, ZBB16, ZH12, ZZZ +19, ZCWX18, dSH19, vSGP10, JCHT18, ZSB +11]. Analytic [Boz18, MDTD13, NF18, SZX13a, SZX13b, TSH +19, MY17b]. Analytical [CCR18, CCB15, HNWF07, HNWF12, HH17, LBGS16, SFG +17, WOH18, CHC +13, FBY +17, GRN19, HH16a, KN17, KTSG11, MK13a, Pon11, Pop18, ZWF15]. analytics [JZL +17]. analyze [LP11c, OVPK15, QLQ11, RLG14, YKO +11, dVAG16]. analyzer [JJW +14, LC12, PVZ13]. Analyzing [BGS +19, BD11, MRB14, BCP +10, HPT17, LZS +17, PHT17, SWA13, WES13]. anapole [ZPP +16]. anatase [HRL11]. and/or [KB10, Pog10]. androstenedione [VCM15]. angle [CKP10, GBFD12, XML +15]. angle-dependent [CKP10]. angles [BKLA13, EJ13, FZY +12, GREA11, KTK17, LDH +14, OZ14, YZ16]. angular [BBG +18b, ENKK +17]. anharmonic [Kow11, SSWX14]. anhydrase [SSP +13]. anhydrates [RB12]. aniline [PLP +16]. Anion [TT18, CG15, KSNT19, LC10, uLhY11, LCC18, SC18a, SDF12]. Anionic [BHP19, AM19a, AM19b, GZZ12, GWPJ11, HPL13, JCP14, QZ10b, YZR +15]. anionic-water [JCP14]. anions [PV12, RDT14, RJS17, ZWY +10b, ZYL +12]. anisotropic [ANO10a, CAT +13, EPH +13, ENKK +17, NLP +16, SLX +15, SN10]. anisotropy [BP18, CGP12, LPLB16, ZLZ14]. ANN [XWW +11, ZDW18]. ANN-based [ZDW18]. annealing
annihilation [BL12].
annulated [RS17a].
anode [GNI18, YZLZ19].
Anomerization [SM17].
anomers [HH11].
ansa [OSA19].
ansa-zirconocene [OSA19].
anza-zirconocene/borate [OSA19].
ansatz [Bou14, WGA18].
answer [SJWE10, Tan19].
ant [ZsA10].
antagonists [LLL+10].
antibiotics [PG15].
antibody [UNT16].
antiaromatic [TDKT10].
antibodies [HH15, ZDW18].
anticooperativity [TDT19].
antiferromagnetic [ZB18].
antitubercular [TD10].
AO [YOPB16].
AOFORCE [vW11].
APBS [UHH+11].
API [LAS+14, ZW18].
AppA [XBSS19].
Applicability [MAK+14, DI11, GHL17, GKR13, HH15, JZZM14, KMS+19, Ray13, RKG11, VHS+19].
applicable [CL16, WGL+11].
Application [AFBR17, BAMR13, BPE16, DAG19, GCCM15, HTS15, LDG+15, MBA11, MTS+19, MHI10, OL13, PAK15, RVP+11, SMP17a, SRS14, SCI7, SDL14, SMM+18, Tak18, VKTRJ15, WH11, WFS19, ZsA10, vSGP10, CSAdOM17, CJPCTC18, DGPMD14, Elk16, GLB16, GFG11, GWC16, HYSF19, IUK+11, KTG19, KSY18, KSK11, LLHM16, LP11a, LLLC11, LVG13c, MTD13, MdOQ18, PHC13, RZG+13, RCM+13b, SMDP18, SN16a, SLX+15, SYH12, VV14, VKC10, WCDM11, You10, APFI13, BD11, CZNA11, Fer13b, Fer13a, FCQGM12, GAI13, HYUS11, KUDG12, MCC1, Pet11, PW12, SPZP19, TSZQ12].
Applications [KGHC15, LCPS13, LCA17, SPR18, APK14, CGP011, EVR18, Fel10, GBFD12, HZY+10, HCD+10, IO13b, KKO+16, uLhY11, JLR+12, MG11, NS18, SSSM15, SGM+13, ISP+10].
approached [BLG11, CTP13, GKR13, KKR+13, LTT16, PM18b, Ray13, RKG11, BZSM15].
Approach [KB11a, ZSLL17, CC11].
Approach-an [KKH18].
approaches [BP18, BH13, CME11, DBM+17, ECZWD17, HBI+17, IT19, LSH+11, RDDJ17, RR15, VLB+10, YJ11, ZDT18].
Approximate [LZLC13].
Approximation [AO10, Boz18, Cas13, HH17, Kid19, Sch12, WHM10, WDKT19, YD17, YN15].

Base [GBM18, BH13, BZH14, DKT13, DSB^+19, FD14, GA18, HvM12, LZH^+11, LW11, ONTTL16, SZSZ16, VMP^+17, WXY14, YKH^+10, ZLL^+10, ZLHH14].
base-catalyzed [WXY14]. Based [AIM^+18, CSM16, CPK19, L19, SN16b, YKNN19, AMGB10, ALK^+15, AM10, AWF^+18, AO10, BCSC1^+13, BAMR13, BPE16, BMPML^+13, BHR15, BMD19, CFM^+19, CC18c, CQA19, CGPP11, CSC^+18, CDS16, COH19, CH10, CGBK13, CB11b, DK11, DVVP14, DH14, Dil15, DJX^+11b, DJX^+11a, DFF^+15, DPB^+12, DXL^+10, DCS15, DDM^+15, EFAC13, ESPT16, EV14, EBK13, EP15, EBPK17a, EB18, FCL^+10, FCOGM12, FCPJM14, FHZA^+18, FMG12, Fra15, Fra16, GLB16, GHL17, Gar12, GJMPAM^+14, GJ15^+19, GBVA11, GC18, GVP^+10, GWW19, GNI18, GSS13, GBSE11, GZ14, GKB15b, HKRS11, HS11, HLS12, HH11, HTS15, HW19, HZY^+10, HSW^+19, HPL^+18, HKR12, HB14, HEMCZE^+14, HSB^+11, HYUS11, HM13, HLWD15, ISN13, IN19, ISM18, JJJW^+14, JLCA17, KS18, KGHC15, KZZ^+16, KLZ^+18, KNE11a, KC14, KSHP^+19, KP11, KKH18]. based [LSL^+19, LFB14, LZ11, LM18a, LDB^+17, LMZX11a, LMZ^+11b, LWL^+11, LLZA12, LSH^+11, LZS^+17, LZZM19, LTA^+11, LGKS17, MDTD16, MZ11, MMM^+16, Man19a, MSY19, MC10, MP19a, MA16, MS13, MdOdQ18, MGCC19, MPNS13, MMZW14, MAP18, MFR^+17, MO15, MNNK10b, NB19, NC12, NC13, NC14, NMI19, NJX^+10, NG10, OVPK15, OZLSBH12, PRP15, PLZ17, PC11, PSC11, PBBP11, PN13, PKIC11, PPJ14, PLH16, PBE16.
based on [CDS16]. Bases [WBKS19, CWZB10, KASH14, LRVM18, MSLS10, SC18b, SBW12, WGA18, ZT14, dCLFGL13, dSVdM16, dVZ17, FAS+18, NKJ16, WTD+19, ZDL18, dLvNC18a, dLvNC18b].
[KRSC12, HLH+12, Hug12, LH11, LJ+12, SKKS13]. beta-barrel [LJR+12].
beta-complex [SKKS13]. Beta-decomposition [KRSC12]. beta-peptides
[HLH+12]. Bethe [KK17b]. better
[AF14, BM12, JT18, KDS17, yOaCG10, XHLH16]. Between
[ELKE19, ALW+10, ASL+11, AR10, ACS12, AHK+19, BSF18, BSD18,
CCCLRQ14, CC18b, CZH12, CQFC10, CC0H14, CB11a, dRCFGRB18,
DHF+11, Den12, FD14, FC16, GYX+10, GO13, Gav12, GKSS14, HSJ18,
HTY19, HvM16, HvM17, HHWL17, Jab18a, Jia19, KTT16, KHWB17,
KPH+19, LDJ+10, LLL+11, LW11, LYL16, LWL+16, LvG13b, Lüc14, MS17,
MUGNVJ+18, MSSP17, MdVBD18, OHNK11, OCL11, PRJ+17, PL14,
RSRR15, SBW12, TTR+12, TSN16, WCT+11, WFZ+18, WDS+19, Wei12b,
YHG+11, YK15, YPH+19, YDGZ15, ZY14, Z18B, ZBMZH15]. Beyond
[PNW+16, JND+19, RLA18, SCOJ13]. BH [LBTV11, LBTV12, Kop15b].
Bi [ATIP18, RDT14, DM15, VIT+15, HSJ18]. bias [KEMP17, KS12].
[BEM+14, BEPM14, WFL+19]. Big [WDKT19, MPA12]. big-bang [MPA12].
BiH [HSJ18]. Bilayer
[vRWGS17, II18, KLN16, RBOH11, SLX+15, WHAS+10, WHAS+16].
Bilayers [BPPS19, BPPS17, GBL+11, PVM10, PS10, RI10, TG12a].
Bimetallic [GEP+14, DAdGR15, GTT10, KKPT11, SIT18]. bimolecular
[CSAdOM17]. binary [Hua16, LAS+14]. Binding [AIM+18, ELKE19,
FPB12, GRS15, HVS16, KJDB12, NN19, SSP+13, SMD18, YKNN19, ZP13,
AALCM11, ALW+10, ABD11, AS10, AC11a, ACS12, BHH14, BTMS12,
BVHL17, BEL+11, CBP+15, ČMD13, CLA16, CIKT13, CZY11, CS17,
CZAF17, CHR+12b, CHR+12a, CPK12, CXD+19, DFL+11, DS12b,
DVVP14, DAB16, DPOS16, ETLRS17, GHK12, GDV17, GWZ15, GEP+14,
GPc+16, GJ+17, HKY+13, HDM+19, HPL3, HNWF07, HNWF12, HG13,
HHLW17, ISP+10, JCP14, JZ12, KZZ+16, KTO11, KTO13, KDT+12,
Lar12, LL10b, LW11a, LW11, LCA17, LSB10, MSY19, MLZZ12,
MLN+18, MGWR12, MSAK12, MAP18, MFR+17, MNNK10a, NST14,
NHN16, NW17, NZM18, NFG+13, NF17, NN18, NO16, NKK+16, OBW12,
Oht16, OHNK11, ORS16, OCLM14, OOT15, PGCT+12, PBLd12, PGS+15,
Pla11, RLDJ17, RCR+16, RDDS10, RAR+11, RO14b, RZ16, RF15, Rez19].
binding [SPS+12, SRA17, SOD+11, STM+15, TYZ+16, TJ19, TS15a,
UNT16, VV13, Vor10, VM11, VHS+19, WS10, WNP+16, WLLH18,
WWW19, WL14, XHLH16, YZ15a, YZZ16, YXZ13, YHH+13, Z14b,
ZJZM13, ZY1Z14, ZGX+13, dRBO13]. binding-based [MAP18].
binding-site [SP+10]. binds [XHLH16]. BINOL [HPT16a].
BINOL-phosphoric [HPT16a]. Binor [WJX+10]. Binor-S [WJX+10].
binuclear [KMS+19, LZZT10]. bio [MSvG12, RZ16]. biochemical
[DGSVGM19, RB12]. biofuels [LGC19]. bioisosterism [EdOdS18].
BiOLayer [JAH+17]. biological
[BHB12, Ben17, CLK11, DLL+10, DMN15, GREAA11, GFFSD17, GLM+17,
bonding-induced [YLZ+10].

bonding/back [PKK17]. bonding/back-bonding [PKK17]. Bonds [ELKE19, JLLW19, WFZ+18, BT18, CXD+19, DGB+13, ED15, FPRS14, Gra18, HHI+15, Jab14, JJJ+16, LZH+11, LZL+15b, LZY12b, LDG+15, OOK11, PGI+19, Roh+13, SM16a, SK13, SJ16, TDT+19, WS19, XMA+19, YLT+19, YLL11, YKH+15, YJ+17, ZLY+16, Jab18b, YLZ+19]. BonnMag [BBG+18b].


C [LdSRR16, LTR18, LAHS16, LLD17, LCWW10, LWD13, MLQ+12, MCK17a, MCK17b, NDK18, PMG+16, RLA+11, Sak18, SKMS13, STS+10, SBW12, Tak11, UT15, WCY+11, WWKS16, YZZ+17, ZYG+14, ZLY+16, ZLX+19, BS16a, VAMS14, AM19a, Ben17, BWKW10a, BS16b, BH13, CG12, ED15, FL15, GWT+17, GMSV14, GZ12, HJ13, HS16, IMK+16, JLS+10, JLLW19, KV14, KMT+19, KP10, LFB14, LCC17, LDH+14, MSV16, MH11, MSPC19, Niz13, OPR16, PTK11, Pie14, PZBA13, RWR+13, SNDK16, TFQ+10, TFQ+11, TS15a, TKCN19, VAR12, VED10, WK10a, WLW+10, WS10, WWT19, WL14, WTH+16, Yes12, Yes15, YDGZ15, ZZZ+19, ZZL19].

EBK13, EB18, FAA15, FRC18, FA18, FE14, GRARO+14, GA18, GMO16, HASR+12, HYL+11, HS14a, HB14, HSH15, Hel13, HG10, HG13, HBL12, HYS11, HGW18, Ibr17, IMS18, ISM18, JCG+11, KK17a, KB10, KKNN11, KGHK12, KMS+19, KKR+13, KERY+16, KFT18, KCPMG12, KKL+13, KSH+17, KKH18, LedOLdV17, LRVM18, LOB18, LMZ11a, LCH10, Lyc+13, LCA17, LvG13b, LCK+18, LCM+14, Lun12, MK17, MK19, MUGNVJ+18, MLN+18, MCLD10, MEH18, MCK17a, MCK17b, NWW17, NZM18, NLL19, OLA15, OOT15, OZLSBH12, PBLdS12, PTK11, PHK14, POB13, PBBP11, PDG+16, PN13, PGW+17, RAR+11, RLZ+18, RHT+15, RLD12, RR11, REV+17, RI10, RK15, SH15, SRSLO15, SP13, SPF+18, SS16b, SCW11, SWPR11, SRS14, SMP17b, SDMS13, SHB17, SKTT11, SPZP18b, SPZP19, TLdG+12, TNY18, TS10a, TN19b, UHH+18, VLB+10, VKAM12, VKNT16, VHR16, VFRAR16, VMPS17, VI17, WC13, WSZW15, WHK+12, WTH+16, WGA18, WXY+14, YYW+16, YDJ17, YN15, YJ19, ZRCC11, ZLT13, ZLZ14, ZWMW10, ZH12, MSC19, NQB19. calculations [OLA15, OOT15, OZLSBH12, PBLdS12, PTK11, PHK14, POB13, PBBP11, PDG+16, PN13, PGW+17, RAR+11, RLZ+18, RHT+15, RLD12, RR11, REV+17, RI10, RK15, SH15, SRSLO15, SP13, SPF+18, SS16b, SCW11, SWPR11, SRS14, SMP17b, SDMS13, SHB17, SKTT11, SPZP18b, SPZP19, TLdG+12, TNY18, TS10a, TN19b, UHH+18, VLB+10, VKAM12, VKNT16, VHR16, VFRAR16, VMPS17, VI17, WC13, WSZW15, WHK+12, WTH+16, WGA18, WXY14, YYW+14, YYJ+16, YDJ17, YN15, YJ19, ZRCC11, ZLT13, ZLZ14, ZWMW10, ZH12, MSC19, NQB19].
calculated [VVLG17]. Calibrations [CBP14, DDM+15].
calix [GMASBF16, PRRT+10, YCGA10, ZWY+10a, ZWS+10, GMASBF16]. Call [ZPF14].
calorimeter [JLS18]. Can [ASMS10, IMSR18, KV15b, LZW+11, NH19, PLAG11, SHL+13, SPZP18a, CIKT13, LCB10, TCPPC14, Zha12b].
capacity [KOP+14, PGC12, WK10a, WK12]. capillary [NFPD13].
caps [WDS+19]. capture [GLZ17, SMD18]. Car [DL19, KCK+15].
CARB1/TIP3P [SA10]. carbazole [JYS+12, SLC+17, YJN+11].
carbazole-based [SLC+17]. carbazole-fluorene [YJN+11]. CarbBuilder [KSW16]. carbene [CWT+12, LXZ+10, TCPPC14, WSL1, WS12, YJ19, dSDLBNB17].
carbenes [BAD+19, BSDP16, KYKR15, RF15]. carbocation [ONTTL16].
carbon-beryllium [CME11]. carbon-carbon [KGJ19].
carbonyls [SSX+14]. carboranes [HJ13]. carboxybetaine [DQ16].
carboxylates [AARP17, RVM19]. carboxylation [CKG18, DGSVGVM19].
carboxylic [LPMT17, RB12, dSH19]. card [SR11].
Carlo [HMM11, NQB19, Aou16, BFH+13, CLK11, CG12, CTP13, CAP17,
DMN15, FFA14, GP12, GPM17, HFSO12, Hes19, HMM10, HYUS11, HQC16,
HHBY10, IHJ+13, LPK16, LMZ11a, LZ12, MS16, MBRC16, MOS12,
NDW15, OPBR17, PSS14, PS13, Pon10, PHH+12, RHNN10, RdA12,
SCOJ13, SAGC16, SMRM+17, SSP19a, SE14, SE14, UU12, YO19, ZLM+15, ZW17].
Carlo/Brownian [DMN15]. Carlo/molecular [RdA12].
caroabiose [YSRSS10].
carotenoids [PVAM16].
carrabiose [YSRSS10].
carrier [SFDE16].
carriers [GMASBF16, UGK18].
cartesian [REH13, FHMB15, AlQ19, Elk16].
caryolene [ONTTL16]. caryolene-forming [ONTTL16].
CAS [KMS+19, MH11]. cascade [HS17b, ONTTL16, ZZWT12].
cascaded [LZL+15a]. Case [BMD19, Alg17, ASMS10, AM19a, AM19b, BM12, BG13,
CCLP12, CB11e, DSB+19, DOM+11, DS12a, EFOD13, EOA+11, GH10,
GKR13, GpdC+16, HSH15, KB13, LPAS11, LP11a, LT13, MIS+15, OME16,
PG18, PVAM16, Ray13, RVM19, Rod13, RKG11, RCM+13b, RJS17, SRF+17,
SC18a, SPZP18b, TLA10, VKNT6, WDS+19, ZTH+15, ZAR+11]. cases
[GREA11]. CASPT2 [LWGZ15, SGWA17, VFRAR16, WGA18].
Cassandra [SMRM+17].
CASSCF [KSHP+19, KKL+13, LWGZ15, NH19, SGWA17].
CASSCF/MC [KKL+13].
CASSCF/MC-XQDPT2 [KKL+13]. CAST [GBW+14]. catalysis [Can10,
Can11, EvRC+18, GSMZ19, KK19, LHMM11, MG14, RNS19, WFL+19].
catalyst [BEM14, DK19, DSHLM18, LLC17, OSA19, RLZ+18, WWT19,
Y2Z15b, ZW11, ZW11, ZW11].
catalysts [AHK+19, BEPM14, GSMZ19, JAB16, MPJ+19, NJX+10, WJX+10].
Catalytic [YMY+19, AHK+19, GHL17, GA19, KV15b, ONTTL16, SJD14,
SLY+10, SOYCL12, TM18, UKS11, WZQW10, dSDdAR10]. catalyzed
[AS11, BF19b, CYY+17, CJC10, CPLL11, HPT1a, HDB15, HJLV16,
KSO+19, KB13, KT12, MUN+19, MRC+18, MG15, MTS+19, QLYL10,
TLA10, Tsi17, VCM15, WCWW11, WFL+19, WWT19, WX14, XLY10,
YXZZ17, YZ17, YZLZ18, dSDdAR10, dSDdBR17, dCDP15].
catastrophe [ABDGN12, GNDA+12]. catechol [PBLdS12].
catechol-O-methyltransferase [PBLdS12]. Catenanes [LAHS16].
cathepsin [ETLS17]. cathode [SMIN+19]. cation [CCCLCGRO14,
CGPP11, DLHLM12, DDM+15, MUN+19, RMGB11, SSGS15, ZYL+12].
Cationic [HJ13, SC18a, WJX+10]. Cations
[N19, SB19, C18b, KGR+16, LCL+10, LdSRR16, LTR18, PVS12,
SB+17, Tac17, THP+15, ZWY+10a, ZWS+10].
cations/nucleobases [CC18b]. caused [GDV17].
caveolin [PG19]. caveolin-1 [PG19]. cavitand [CC18a].
cavities [HRB+17, ZSB+16]. cavities/vacancies [HRB+17].
cavity [KD18, ZWS+10].
CAYS [SDZ17]. CB [BTMS12, CC18a, ILKR11].
CC3 [LZ14]. ccCA [RJWW12]. CCSD
CeO [LLW19]. CEPA [Sch12, SB14]. ceramics [RKB+14].


[vRWS17, BFH+13, CHKR10, DMD+18, HAL14, KV14, KLS10, KML10, LPS+13, LZGS11, LP11b, LvG13a, LZLMP16, OZ14, PD12, PS10, QZ11, SA13, SISK10, SZBM13, TSN16, DKV18]. chains

[AFSW16, FPI1a, JW10, LZZ14, NPP13, PLA11, PLH16, TLdG+12, TS15b].


[HGY15, KHWB17, ASW19, HLvdV13]. challenging

[CAP17, DSB+19, VT14, WLF11]. change [EMD17, OSA19]. changes

[GDV17, GBS+17, HB15, LK13, MJLV14b, MO17, PsDC18, RO14b, YZGS14b].

Changing [XVN17, LLvG10]. channel

[HYYZ13, PVL+13, SBFB17, SY16b, TCX+13]. channels

[KC13a, LL10c, NS18, OKIS17, TO19]. character

[Ali18, BMB13, Cas14, Br17, LCK+18, RIJ+11, VSH19, YSSB12]. characteristics

[DSL16, Gav12, LT14, Mat14, RDT14, TZ11]. Characterization [DDP+18, VT14, XWSW13, CBP+15, DGL+13, GBW+14, GZZ12, Kop15b, MJBM12, MPA10, RNP13, ZYG+14]. characterize [MGCC19]. Characterizing [HL11, PRSG13, Sh12, Yu12b].

characters [LSH+11, ZLL+10]. Charge [CMF+17, JM11, RDT14, SFDE16, VV19, AWF+18, AS15b, ANH+11, ALH+10, BCSCJ+13, BE16, CS14, CBTZ16, CMS13, Cor17, DS12a, DWR17, DADGR15, EFAC13, ENKK+17, GMG+10, HLWD15, JCGVPHT17, JZM14, Jia19, Kan15, KVR10, LLLM11, LEP+10, LBDP12, MSV16, MCF+18, MHRR11, MPBJ11, NN18, OBW12,
PL14, PTB+15, RSSG18, RO14b, Rez19, Ric16, REL17, SPS+12, SFM+18, SSGS15, SMiN+19, SMP17a, SFLG+17, SLC+17, TN10, TKNN10, UT15, UGK18, VPR10, VAR12, VL17b, WCT+11, WWCL15, YKO+11, YWZ14, YLZ+10, YJ17, YFH+19, ZDM13, ZL19, dSH19, dLC17]. charge-assisted [SSGS15]. charge-inverted [UT15, YJ17]. Charge-transfer [JM11, ANH+11, EFAC13, YLZ+10]. charge-transport [HLWD15].


Chemical [BLG10, BCP+10, BGS+19, JCGVPHT17, OSI+19, OM12, SLLL13, VGTL16, ALK+15, ASS+17, AAC+16, APA+14, Bac12, BPC19, Ben17, Bou14, Cam15, CKG18, CHP11, DKE+17, DDF+18, DS12a, DI11, DB12, Dra19, EO+11, FB10, FVB10, GH10, GLW19, GGM+12, GPGSM11, GPGSM12, HPT+16b, HHDC16, HJ13, Ihl12, JKS+16, KV12, KASH14, KP11, LK11, LZH+11, Li4a, Li4b, MDTD13, MDTD16, Man19b, MN15, MTS+19, MAPB10, MSvG12, MSSP17, MFR+11, MMJ10, MH10, NCV10, NC13, OK1S17, OKY18, OSH17, ONTTL16, OC14, PTK11, PGDo+16, Pie14, PBG17, RRFV+18, RK15, RSKG14, SRA17, SLT14, SFM+18, SOJ13, SEF+16, SKMS13, SHB17, TLA10, TG12b, TEDT18, TR12, UD12, VBD11, VDMA13, WBT10, WCT+11, WF16, Wei12b, WL14, Wu10, WDP+12, YZ15a, YB16, YZ14, ZBB16, ZLT14].


chemist [DHE+12]. Chemistry [Ano10b, Ano15-59, Cam19, HJG09, KKGW19, Spr10, ZLX+19, Ali11, BRP+12, BGR13, CBH14, CD19, DDM+15, FLM11, GHV17, HSN+18, IGK16, JBB+11, KTN10, LBC+19, LKI6a, MP19c, OZLSBH12, PNV+16, PPUBGD10, RZG+13, Rez16, REL+14, TKNN10, TF15, UKD+18, VVP12, VV14, WDIY13, ZVY+15, GS16, MFEM16, XFG+16].

Chloroammonium [VVMY18]. chloroform
[GC11, WG12]. chloroform-to-water [WG12]. CHOC [LHWH14]. choice
[LvG13b, Mor15, NCV10, SPZP18b, TLA10, WGA18]. Cholesky
[GCW16, PS17]. Cholesterol [BPSP19, BPSP17, RBOH11]. choline [PP19].
choline-O-sulfate [PP19], chondroitin [CHKR10]. chondroitin-6-sulfate [CHKR10].
Chou [FZL15, GRIL11, GRIL12, ZHHX11]. chromophore
[GA18, PGW17, SGWA17]. chromophores [SGDT10, UD12]. CI
[CME11, EFAC13, EPS16, FE14, IN13, KMS19, KSHP19, MN19, PH10b,
SRF17, SCF19]. circuits [RVB12]. circular
[HNHR13, SE15, SB13, SB15]. circularly [SE15]. Cis-
[CSM16, MSB16, WvRSM14, WS19, ZLHH14]. Cis-
[CSM16, MSB16, WvRSM14]. CISS [dALdS15]. cisplatin
[dRCFGB18, CK17, PML12]. CI [ATP18, ASS17, CXS10, EPH15,
GPK16, KKR13, LDJ10, LLL11, LZJ11, LGW12, PMG16, Rab12,
RvdMB16, Sak18, TFQ10, TFQ11, Tsi19, TDT19, WGN16, WGLG16,
YS13, ZCK16, ZLLL12, CSNC18, JGC10, JLS10, JLH14, LZL15b,
MSPC19, W LH12, WLF19, ZWY10]. Clar [KDS17]. Clarifying
[RML15]. class [DWL11, HHWL17, LD18, ZLW10]. classical
[Aki16, BEM14, DIF11, GA19, HS14a, HLvdV13, LRvdSM15, LM18a,
LPE10, LM18b, MS15, PVAM16, Ras17, RTS13, RO14b, SM14b, SAK19,
WKC10b, WG14, Yu12a, ZM10]. classification [EP15, UT15]. classifier
[YHH13]. classifying [TO19]. Clay [HBH19, BBH17]. CIC [KJ10].
cleaning [YR13]. cleavage [HEM17, MS11]. click [TKXT13]. CLL
[dACP12]. CINH [VVMY18]. close [BLZ13, MK17, RS13]. Closed
[CY110, MA16, MS12, WW1D4]. closed-shell [MA16, WW1D4]. Clos-
[TF15]. cluspro [XM15]. Cluster [AST16, Hes19, MPNS13, SL17,
ACD13a, ACD13b, AC11b, Avd18, BBG18a, BYE16, Cas14, CCI1c,
DI11, DM15, FF11, GNGCA10, GMG10, GA18, GS11, HAGK10, HSB19,
HS15, Höf14, HGCGCR16, HBI17, Les19, MC12, MG14, NLL19, Oht16,
PGB15, PB14, PMT16, RS14, RLZ18, SB11, SLLL13, SM17, TLdG12,
TN18, TTn19, VIT15, VV15, WC13, XTN18]. Cluster-based [MPNS13].
cluster-continuum [WC13]. cluster-expansion [HAGK10].
cluster-in-molecule [NLL19]. cluster/configuration [FF11].
cluster/Kohn [VV14]. clustering
[BSZ12, LZZ17, PL19, YZ15a, ZSS13]. Clusters
[NSN19, SC17, TT18, AFPI13, ATIP18, AF14, ANo11, ASS10, AC12, BPM15,
BACSCJ10, CJL13, CZZL19, DAG19, DH11, FCW14, GTT10, GC18,
GRD10, GAMAC14, GZZ12, GBGR16, GBG19, HS14a, HS16b,
HDM19, Hsu14, JM11, JCP14, JHMB10, JHMB11, JGC11, KD10,
KKPT11, KOP14, KSNT19, KDB13, LTZTV10, LK13, LZZ11, LCH15,
LCWW10, MCS11, Man19b, MPA10, MP10, MP13, MBFG15, MBRC16,
MCAY15, NC13, NC14, OKY18, PM18b, QZ10b, Rab12, RGVC19, RB13,
commercial [TF15]. Common [HTS17, RNP13, PH15].
commonly [PGY15, Pie14, PLAG11, SPR+13]. Communication
[PH15, KP10, LAT11]. Communications [CDB10, CDBM11]. CoMnO
[LLL+12]. Comp
[ABB+13, CHR+12b, HNW12, ICS+13, Kne11b, MSK+12]. compact
[RLD12]. compactness [PTB+15]. comparable [Gil11]. Comparative
[GZZM16, GVP+10, LAM19, LAW+16, MJC14, MS13, SPR+13, WYG12,
BT18, BFC13, BS10c, JJB16, RSG18, VMRS17, ZYG+15, CJZS10,
PS10]. compared [SGWA17]. Comparing
[FBEM11, GMPB12, Hug14, MS16, SRF+17, VMPS17, SJC11]. Comparison
[BBG+18a, BK13, BK17b, BVC13, GPM17, MHO18, MVKS10, NFPD13,
NTNY15, OCL11, PGY15, Sch18, SLP+12, ST18, STM+15, TLY+12,
YAS13, dRBO13, AGR11a, BAMR13, BB11b, CDM+15, DLL+10, FED17,
GR11, HCB11, HBI+17, HM13, KDL+12, KMLS10, LLSW14, MJLV14a,
MvBD18, PXXW10, PKK17, PD11, RKGN10, Rob13, RŠRR15, T1G12a,
UD12, VVBL17, WTH+16, WGI2, YLGX14, Kar17, Mat10, SA10, YJ11].
comparisons [BMR11]. compatibility [EOO+16]. compatible
[KYB13, MPBJ11, RO14a, SOYC12, VHA+10]. competing [SLT14].
Competition [HvM16, LLL+15b, HvM17]. Competitive
[ZSL+11, GMBX+16, RLJ17]. compilation [NKJ16]. complementarity
[GPS10, OAN15b]. Complementary [EVR18]. Complete
[SN16b, CSKH15, LYC+13, OAN15a, SPS+12, SCSW13, TCB16].
completeness [Leh15]. completeness-optimization [Leh15]. Complex
[DLT17, HBL12, KKGW19, ANH+11, BLF14, BH19, DK19, DaGDR15,
Dry14, FFA14, GCWS15, HBJ+17, Ish10, KBC12, KMS+19, KGH15,
KPG18, KZP+18b, KSW16, LLL+11, LZJ+11, LL11, LWXC16, MLGB16,
MTS+19, MY17a, MY17b, NH19, NDB18, OME16, OC14,
PPUBGD10, QQLY10, SLT+15, SKKS13, SL17, SYN+12, SPM+19, TDP+12,
TN19b, WKL12, WCW11, WHX+10, WSWD19, ZT14]. compexation
[CBP+15, SNS16]. Complexes
[BF19a, BGS+19, EHSPT16, GP4C+16, SvL18, SKGB13, AvKSP16,
AM11, ASMS10, AK10, AM19a, BCSC13+13, BLFZ13, BLDK+13, BSG+18b,
CSGOA17, CPR18, CWT+12, CMD13, CZH12, CGPP11, CAT+13,
CBDS19, CMS13, CM16, CB11d, DS12b, DLP11, EPB+13, ED15, FHW+11,
FCE15, FPB12, FB14a, GKI5a, GHL17, GPK+16, Gil11, dCGCR19, Gra18,
HDK+12, HSY+11, HK12, HLB15, HRJ+14, HGHP14, HRJ+15, HDPM14,
HG10, HQS19, ITY+19, JRSH14, KT12, KPL13, KTK17, LS11a, LLC+10,
LWL+11, LHWH14, LZZ+15b, LDZW17, LZX+10, LYSS11, LJJ+11,
MUN+19, MLG18, MC10, MFR+11, MKK+19, OSHG17, OOT15, PCGT+12,
PH14, PM13, PZB13, RRH12, RHPWS13, RLD12, SB10, SZdB19, SLIB12,
SPR+13, SCSM19, SDL14, SGH+16, TLY+12, TS15a, Tru18, TKCN19,
TS10b, Tsi19, VLB+10, VVP12, VVY17, WL14, XMSZ16, YMY+19, YKH15].
complexes [ZCK+16, ZRCC12, ZZZ+12, ZLZ14, ZDX11, ZYW+10b,
ZYW+10a, ZZL19, ZBMZH15, vSGP10]. complexity [GP12, NS15].
concentration [IPAA11], concept [GRL\textsuperscript{+11}, GRL\textsuperscript{+12}, dSVdM\textsuperscript{+16}].
conceptual [DDP\textsuperscript{+18}, vSI\textsuperscript{18}], concerted [LI\textsuperscript{10}], concurrent [HS\textsuperscript{14b}].
condensation [KNE\textsuperscript{11a}, XLY\textsuperscript{10}], condensed [BGL\textsuperscript{+18}, BG\textsubscript{17}, HRB\textsuperscript{+17}, MKK\textsuperscript{+19}, RSLML\textsubscript{12}, VKAM\textsubscript{12}, dSS\textsubscript{12a}, dSS\textsubscript{12b}]. condensed-matter [BGL\textsuperscript{+18}], condensed-phase [MKS\textsuperscript{+19}], condition [AA\textsuperscript{18}, IKN\textsuperscript{13}, MVT\textsubscript{12}, TAC\textsuperscript{+18}, YAO\textsuperscript{18}]. conditional [BMP\textsubscript{13}].
conditions [AA\textsuperscript{18}, BRGN\textsubscript{12}, KB\textsubscript{14a}, MO\textsubscript{15}, MO\textsubscript{17}, NO\textsubscript{16}, SSP\textsubscript{19a}, Sie\textsubscript{15}, SKMS\textsubscript{13}, TC\textsubscript{14}, VECT\textsubscript{12}]. CONDON
[SV\textsubscript{18}, CHC\textsuperscript{+13}, MLC\textsubscript{10}, ML\textsubscript{11}]. conducting [SV\textsubscript{11}]. conduction [KJ\textsubscript{10}]. conductivity [ASL\textsuperscript{+11}]. Conductor [KB\textsubscript{14b}, GRN\textsubscript{19}, KD\textsubscript{18}, SDF\textsuperscript{+17}]. Conductor-like [KB\textsubscript{14b}, GRN\textsubscript{19}, KD\textsubscript{18}, SDF\textsuperscript{+17}]. conductors [MR\textsubscript{14}, NFI\textsuperscript{+16}]. cone [BKL\textsubscript{13}]. confidence [KSM\textsubscript{17}]. Configuration [KKG\textsubscript{19}, SS\textsubscript{13a}, Cas\textsubscript{13}, CTP\textsubscript{17}, EK\textsubscript{17}, FF\textsubscript{11}, FA\textsubscript{18}, GA\textsubscript{14}, GP\textsubscript{11a}, HPT\textsubscript{17}, HBL\textsubscript{12}, LCB\textsubscript{10}, MT\textsubscript{19b}, MIS\textsuperscript{+15}, MCP\textsubscript{18}, ZRCC\textsubscript{11}]. configural [RO\textsuperscript{14a}, WTD\textsuperscript{+19}, WDH\textsubscript{13}]. Confined [NSP\textsubscript{15}, CCR\textsubscript{18}, CDB\textsubscript{10}, FTR\textsubscript{15}, Vy\textsubscript{15}, Vy\textsubscript{16}]. Confinement [CC\textsubscript{18a}, DCL\textsubscript{18b}, TM\textsubscript{16}]. Confining [WR\textsuperscript{+17}]. conformation [AST\textsubscript{15}, CR\textsubscript{19}, EJ\textsubscript{13}, FB\textsubscript{18}, GK\textsubscript{J}, GV\textsubscript{10}, SE\textsubscript{F}]. conformational-dependent [PV\textsubscript{11}]. Conformational [CD\textsubscript{15}, ETL\textsubscript{17}, KRT\textsubscript{10}, LGL\textsubscript{11}, LTA\textsuperscript{+11}, MO\textsubscript{17}, OGL\textsubscript{10}, vRW\textsubscript{17}, AD\textsubscript{10}, BLKP\textsubscript{12}, BD\textsubscript{11}, \(\mathcal{C}\mathcal{M}\textsubscript{13}, \mathcal{D}\mathcal{P}\textsubscript{16}, \mathcal{D}\mathcal{P}\textsubscript{11}, \mathcal{D}\mathcal{S}\textsubscript{18}, \mathcal{F}\mathcal{C}\textsubscript{10}, \mathcal{F}\mathcal{C}\mathcal{O}\mathcal{G}\textsubscript{12}, \mathcal{G}\mathcal{D}\textsubscript{17}, \mathcal{G}\mathcal{O}\textsubscript{13}, \mathcal{G}\mathcal{B}\textsubscript{11}, \mathcal{H}\mathcal{T}\textsubscript{15}, \mathcal{H}\mathcal{Y}\textsubscript{19}, \mathcal{H}\mathcal{D}\textsubscript{17}, \mathcal{H}\mathcal{K}\textsubscript{18}, \mathcal{H}\mathcal{C}\textsubscript{10}, \mathcal{I}\mathcal{M}\textsubscript{11}, \mathcal{N}\mathcal{S}\textsubscript{15}, \mathcal{N}\mathcal{H}\textsubscript{17}, \mathcal{I}\mathcal{S}\textsubscript{13}, \mathcal{S}\mathcal{D}\textsubscript{18}, \mathcal{T}\mathcal{J}\textsubscript{12}, \mathcal{V}\mathcal{Z}\textsubscript{14}, \mathcal{Y}\mathcal{Z}\textsubscript{16}, \mathcal{Y}\mathcal{B}\textsubscript{19}, \mathcal{Y}\mathcal{O}\textsubscript{16}]. conformational-space [AD\textsubscript{10}]. conformationally [AF\textsubscript{13}, CP\textsubscript{15}]. conformations [CC\textsubscript{12b}, DJ\textsubscript{13}, ES\textsubscript{D}\textsubscript{18}, LC\textsubscript{16}, LZZ\textsubscript{14}, NR\textsubscript{11}, O\mathcal{C}\textsubscript{11}, PG\textsubscript{19}, PH\textsubscript{10a}, RV\textsubscript{P}\textsubscript{+11}, ZC\textsubscript{14}, DK\textsubscript{V}\textsubscript{18}]. Conformers [SZ\textsubscript{+18}, BHF\textsubscript{+18}, DB\textsubscript{G}\textsubscript{11}, HH\textsubscript{10}, HH\textsubscript{11}, LG\textsubscript{11}, MS\textsubscript{17}, TCG\textsubscript{18}, VP\textsubscript{19}]. congested [Mv\textsubscript{B}\textsubscript{18}]. conjugate [MS\textsubscript{16}]. Conjugated [RV\textsubscript{+12}, B\mathcal{L}\mathcal{B}\textsubscript{+13}, HDH\textsubscript{15a}, HDH\textsubscript{15b}, HDH\textsubscript{15c}, JYS\textsubscript{+12}, RSG\textsubscript{18}, YJ\textsubscript{+11}, JCH\textsubscript{T}\textsubscript{18}]. conjugating [JD\textsubscript{W}\textsubscript{+19}]. conjunction [CG\textsubscript{19}, LB\textsubscript{H}\textsubscript{+11}, N\mathcal{C}\textsubscript{13}, R\mathcal{G}\textsubscript{N}\textsubscript{10}]. connected [ACD\textsubscript{+13a}, ACD\textsubscript{+13b}, NR\textsubscript{11}, XT\textsubscript{n}\textsubscript{18}]. connection [L\mathcal{U}\textsubscript{c}\textsubscript{14}]. connections [CDC\textsubscript{19}]. Connectivity [ISP\textsubscript{+10}, ZYS\textsubscript{+10}]. Conquer [NN\textsubscript{19}, YKN\textsubscript{19}, BR\textsubscript{P}\textsubscript{+12}, BGR\textsubscript{13}, KKN\textsubscript{11}, KFT\textsubscript{18}, NYH\textsubscript{+17}, NN\textsubscript{18}, N\mathcal{N}\textsubscript{+16}, WX\textsubscript{12}, YN\textsubscript{15}]. consensus [DM\textsubscript{17}, SRA\textsubscript{17}, PLV\textsubscript{+11}]. consequences [KG\textsubscript{15}], conservation [MB\textsubscript{16}], conserved [JD\textsubscript{W}\textsubscript{+19}]. Conserving [PH\textsubscript{17}]. considerable [LLD\textsubscript{17}]. Consideration [Fom\textsubscript{11}]. considerations [SB\textsubscript{G}\textsubscript{P}]. Consistent [LOB\textsubscript{18}, MK\textsubscript{+13}, POB\textsubscript{13}, BK\textsubscript{\(\tilde{S}\)}\textsubscript{+11}, BY\textsubscript{11}, BK\textsubscript{17b}, DK\textsubscript{11}, GB\textsubscript{V}\textsubscript{11}, H\textsubscript{i}\textsubscript{13}, HK\textsubscript{+14}, JSH\textsubscript{16}, KT\textsubscript{10}, KFT\textsubscript{18}, LB\textsubscript{H}\textsubscript{+11}, LC\textsubscript{W}\textsubscript{12}, ON\textsubscript{14}, OLP\textsubscript{19}, Rez\textsubscript{19}].
SPS$^{+12}$, SMP$^{17b}$, SC$^{13}$, TYN$^{15}$, VGV$^{+11}$, YN$^{15}$, ZBG$^{11}$, BLKP$^{12}$].

consistently [IM$^{17}$]. consolidate [BK$^{17c}$]. constant

[AB$^{16a}$, CS$^{14}$, IN$^{19}$, KSK$^{11}$, KN$^{+12}$, KB$^{19}$, MK$^{17}$, MK$^{19}$, PLFS$^{18}$, PS$^{13}$, RAGL$^{11}$, Sak$^{18}$, STM$^{17}$, Vor$^{12}$, WOH$^{16}$, WOH$^{18}$, dACP$^{12}$].

constant-distance [dACP$^{12}$]. constants [AAMD$^{+11}$, CBH$^{14}$, CPK$^{12}$, DSD$^{+11}$, ECZWD$^{17}$, FD$^{14}$, GAI$^{13}$, GKR$^{13}$, MG$^{11}$, OZLSBH$^{12}$, Ray$^{13}$, RSG$^{14}$, RKG$^{11}$, Rui$^{11}$, RRK$^{16}$, SPHF$^{+18}$, SH$^{18a}$, SACdG$^{14}$, TTR$^{+12}$, Tsi$^{14}$, WL$^{14}$, XWW$^{+11}$, YS$^{13}$, ZL$^{+10b}$, ZLL$^{12}$].

Constrained [SL$^{15}$, GREA$^{11}$, GA$^{12}$, VBV$^{13b}$, WBN$^{+13}$]. Constraint [HNyH$^{19}$]. constraints [KB$^{11a}$, OPBR$^{17}$, OZ$^{+13}$]. construct [HH$^{10}$]. constructed [HDL$^{+17}$, Tsi$^{19}$, ZL$^{+16}$]. Constructing [Che$^{17}$, LLH$^{+19}$, HS$^{16b}$, LG$^{11}$, SWA$^{13}$]. Construction [FZL$^{+19}$, AGR$^{11b}$, JCP$^{11}$, KD$^{18}$, KSR$^{17}$, LZX$^{16}$, UIW$^{+10}$, WW$^{14}$, YD$^{17}$]. contact [DBK$^{17}$, LL$^{19b}$, MK$^{13a}$]. contact-assisted [LL$^{19b}$]. contacting [Mau$^{14}$]. contacts [CCCLCGRO$^{14}$, Ham$^{11}$, Kri$^{10}$, PRP$^{15}$, SNDK$^{16}$]. containing [AKMYB$^{18}$, ACD$^{+13a}$, ACD$^{+13b}$, DT$^{19}$, DGL$^{+13}$, GP$^{12}$, GPdC$^{+16}$, HDPM$^{14}$, KL$^{12}$, KGJZ$^{19}$, LDZW$^{17}$, MUGNVJ$^{+18}$, VDVR$^{14}$, YHVM$^{12}$, YDX$^{16}$, ZZL$^{+10b}$, ZLLL$^{12}$]. contaminated [YR$^{13}$].

content [CGBK$^{13}$, GWPJ$^{11}$]. Contents [Ano$^{16-115}$, Ano$^{16-121}$, Ano$^{16-122}$, Ano$^{16-123}$, Ano$^{16-124}$, Ano$^{16-125}$, Ano$^{16-126}$, Ano$^{16-127}$, Ano$^{16-128}$, Ano$^{16-116}$, Ano$^{16-117}$, Ano$^{16-118}$, Ano$^{16-119}$, Ano$^{16-120}$]. context [CBG$^{16}$].

continuation [PJ$^{13}$]. Continuous [Dry$^{14}$, LPLA$^{13}$, PZB$^{13}$, BS$^{19}$, FGM$^{11}$, LBGS$^{16}$]. Continuum [CCR$^{18}$, JJ$^{16}$, ND$^{19}$, ALRM$^{18}$, Cam$^{15}$, CZY$^{11}$, GRN$^{19}$, HZSS$^{17}$, ISO$^{+13}$, LFN$^{+10}$, MCUJ$^{15}$, SK$^{12}$, SK$^{17}$, TNG$^{+10}$, WC$^{13}$, WRHF$^{10}$, XZ$^{11}$]. Contracted [FC$^{18}$, SM$^{18}$]. Contraction [Hes$^{19}$, HSN$^{14}$, STM$^{17}$]. contractions [KK$^{17a}$].

Contributions [JJ$^{13}$, ARRC$^{15}$, BCNH$^{+11}$, CGR$^{16}$, CPN$^{+17}$, ENKK$^{+17}$, WS$^{10}$]. control [BV$^{*12}$, DP$^{16}$, Hel$^{13}$, HH$^{16b}$, KFT$^{18}$, LPLB$^{16}$, SR$^{10}$, XYW$^{+14}$, ZQ$^{14}$]. Controlled [PGK$^{+19}$, VGT$L^{16}$]. Controlled-advancement [PGK$^{+19}$].

Controlling [FWB$^{14}$, NPG$^{+18}$, SS$^{19}$]. convenient [ZGZC$^{19}$]. Conventional [SHL$^{+13}$, BK$^{+11}$].

conventions [BCJC$^{+14}$]. converged [FLM$^{11}$, GR$^{10a}$, KHWB$^{17}$]. Convergence [GS$^{16}$, LT$^{13}$, ZH$^{12}$, ASS$^{10}$, BK$^{+11}$].

converges [SHL$^{11a}$]. Converging [OSR$^{16}$]. Conversion [AIQ$^{19}$, DAP$^{+18}$, LDB$^{+17}$, LZL$^{+15a}$].

converted [ZB$^{18}$]. convex [CLFRO$^{18}$, GWW$^{19}$]. convolution [SZTSM$^{10}$]. convolutional [LHO$^{17}$]. cooperative [DBG$^{11}$, WFL$^{+19}$]. Cooperativity [RS$^{14}$, AF$^{16}$].

coordinate [AMGB$^{10}$, HSN$^{14}$, Hel$^{13}$, LL$^{15}$, LL$^{13a}$, MS$^{10}$, WBN$^{+13}$]. coordinated [Sak$^{18}$]. Coordinates [AIQ$^{19}$, BK$^{15}$, LWK$^{+14}$, MK$^{19}$, NCV$^{10}$, PH$^{10a}$, Sch$^{13}$, VB$^{13b}$, You$^{10}$, ZT$^{14}$]. Coordination [LBC$^{+19}$, ASMS$^{10}$, AHK$^{+19}$, CRC$^{13}$, GBPCC$^{19}$, HS$^{16b}$, HH$^{18}$, KL$^{+18}$, KJ$^{10}$, Mor$^{15}$, SB$^{19}$].
GP11a, KSK11, KNP+12, KKA+18, Kos16, KKH18, LLB+12, LSH+11, LWD13, MG11, MCP18, PLFS18, PS17, Rue11, RRK16, SPHF+18, SH18a, SACdG14, Wu10, YB11, ZTH+15, ZLZ14, ZVvI14, GA19]. **couplings** [CSEMB+16, LK11, LZH+11, YFH+19, ZB18, dVAG16]. **covalency** [HS14a].

**Covalent**

[WBT10, FCCP17, HAI+16, KAR12, MR17, OZS+13, RS13, SFA17].

Ano17-28, Ano17y, Ano17-29, Ano17-30, Ano17-31, Ano17-32, Ano17-33, Ano17-34, Ano17y, Ano17-39, Ano17r, Ano17s, Ano18a, Ano18c, Ano18b, Ano18e, Ano18f, Ano18g, Ano18h, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18o, Ano18p, Ano18q, Ano18r, Ano18s, Ano18v, Ano18w, Ano18x, Ano18y, Ano18z, Ano18-27, Ano18-28, Ano18-30, Ano18-31, Ano18-32, Ano18-33, Ano18-34, Ano18-35, Ano18-36, Ano18-37, Ano18-38, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h].

Cover


criteria [MvBD18]. criterion [dLvNC18a]. critical [HEMCZE+14, KCK+15, LTT16, MLZZ12, Wei12a, Wei12b, dLvNC18a].

CrMnAs [LKZM18]. cross

[HPT+16b, HBL12, Lun12, MY17a, MY17b, WMW+10, ZHS+18, dCLFGL13]. cross-boundary [Lun12]. cross-platform [HPT+16b]. cross-section [dCLFGL13]. crossing [LLSW14, QCR12]. crossover [CSS17, KV14, MK17, SHMO11, VFRAR16]. crotonaldehyde [KK19].

crowded [MH17]. crown [AvKSP16, HLB15, MWJ+11].

crown/ammonium [AvKSP16]. CrWO [WMW11]. cryo [MKM+17].

cryo-EM [MKM+17]. cryptands [EHT19]. CRYSPLOT [BPC19]. Crystal [FDCJG18, Krii0, VM11, ASL+11, BCSCJ+13, BCJC+14, Elk16, GMG+10, HB14, HJ10, MCAC+16, NHF+10, NTNY15, SPZP18b, VMV19, OPB+12, CPR18].


CTOCD [PC14]. Cu

[LLX+19, NGAS17, Rab12, RHT+15, SIT18, TS15b, WRG+17, AMK11, CR14, CRMD13, GEP+14, HSH15, MLG18, Mor15, PGS+15, PXXW10, PH12, RHT+15, SB10, TNI+19a, WGN+16, WGLG+16, XP13, ZRCC11, ZSWL12].

Cu-O [ZRC11]. Cu-ZSM-5 [Mor15]. Cu2II [WGLG+16]. Cuby [Rez16].


curcumin [AMK11]. Curie [WMW11]. curing [LPMT17, PPH+14].

Current [ATM18, NS17, ABM+15, ATIP18, BL19, FNSF+11, GWT+17, HBLCCCG15, PCLL11, PL18, PZM15, Vik11]. current-density [Vik11].

currents [CPN+17, RVB+12]. Curvature [LPLS16, RR12, NW17].


cyanide-chemosensing [LZH11]. cyanides [PGS+15].

cyanide [LZH11]. cyanides [PGS+15].

cyanobacteria [RCM+13a, RML+15]. Cyanovirin [VM11].

Cyclobutadiene [SFM14, MCC11]. cyclocized [QZ10a].

cycloadditions [YS13]. Cyclobutadiene [SFM14, MCC11].

Cyclopentadienes [LZH16].

cycloadditions [YS13].

cycloadditions [YS13].

cycloadditions [YS13].

cycloadditions [YS13].

D [LWD13, OZLSBH12, RSKG14, SPHF+18, UT14, GBG+19, MP19b, YZ15b, AKMT11, BKWK10a, BKWK10b, BKHW19, CTK16, MA16, MTT+14, MH11, MSP17, MI10, NN19, PSS14, PZBA13, Pop18, RSGK14, SWW+19, TQ+10, TJJ19, UT15, VVMY18, YJN+11, YDL+10, ZLY+16, dLvNC18b, TS15b, YOPB16].

cyclizations [AARP17, DH14].

cyclizations [AARP17, DH14].

Cytochrome [EH13, BS16a, MRR11, SLY+10, SOYC12, TN10, TDP+12, VCM15].

cytosine [JS17a, LZH+11, ZZY+16].

cytosine [JS17a, LZH+11, ZZY+16].
decomposition-based \[\text{KNE11a}\]. \text{decouples} \[\text{FM10}\]. \text{decoy}

\[\text{HYMZ16, LS11a, PHDH13, UCFR16}\]. \text{decoys} \[\text{BSZ+12, MP11}\]. \text{decrease}

\[\text{DLZ15, SLY+10}\]. \text{dedicated} \[\text{CPRS18, ZRCC11}\]. \text{Deep}

\[\text{GHV17, TO19, GFPSD17, HPL+18, LHO17, LDH+14, WZWW18}\]. \text{deeper}

\[\text{VIT+15}\]. \text{DeepIon} \[\text{TO19}\]. \text{defects} \[\text{HYL+11}\]. \text{Deformed} \[\text{CSAdOM17, TFQ+10}\]. \text{degree}

\[\text{JYC+16}\]. \text{Definitive} \[\text{TCGNT18}\]. \text{Deformation}

\[\text{WYL+15, Gav12, MRB14, WCY+11, WCT+11, dLC17}\]. \text{defective}

\[\text{ZWP11}\]. \text{deficient} \[\text{YLL11}\]. \text{defined}

\[\text{JJAB16, Man19a, GY10}\]. \text{defining}

\[\text{HH18}\]. \text{definitions}

\[\text{JYC+16}\]. \text{Demystifying} \[\text{KKGW19}\]. \text{Denaturation}

\[\text{IPAA11, FMG12}\]. \text{Dendrimer}

\[\text{MJBM12}\]. \text{dendrimers}

\[\text{CAD16, HDHL15a, HDHL15b, HDHL15c}\]. \text{Deng}

\[\text{Ano12u}\]. \text{dense} \[\text{ASK18}\]. \text{Densities}

\[\text{ATM18, ATIP18, HGCCGR+16, LP11c, MA16, REL17, UCRL18, dLC17}\]. \text{Density}

\[\text{AMK11, BS19, BHB19, CD13, CWHH11, CKH19, FPV13, FD16, GMBM18, GNGCA10, GWPJ11, INT18, JYS+12, KKPT11, LBS16, LGW12, LL+19, LBTY12, LPM17, MP19b, MWJ+11, MAP18, NN19, Oht16, PPH+14, RB12, RSLML12, TS10b, UvSvdWK19, WDLG12, WGN+16, YJ11, YKN19, ZLZ14, ZYG+14, ZYW+10b, ZYW+10a, dSD12a, ALK+15, Ali18, ASW19, Ano15-59, AG12, ASS10, BY11, BBG+13, BL19, Ben17, Boc18, BII+11, BZB+13, BG13, CHG+16, CRZ+18, CDB10, CR14, CA10, CEB015, CC18c, CCR16, CKH17, CSXX17, CC11, CAP17, CNK97, CPL11, CXD+19, CB11d, DAP+18, DH17, DWC17, Di15, DSAS19, ED15, EP12, FED17, FCPJM14, GAI14, GHL17, GZL+12, GWJR18, GMG+10, GSS13, Gra15, GEG11, GAI+17, Han11, HNW07, HNW12, HPT17, HEMCZE+14, HLBLCCG15, HRMAL+13, HH16a, HH17\]. \text{density}

\[\text{Hil13, Hs14, HG10, HOK17, IKN13, IM17, JCP14, JZ14, JU16, KD10, KB10, KSSH13, KOP+14, KGHK12, KB13, KZZ+16, KLN12, KYG+15, LL15, LRVM18, LCM12, LAM19, LBTV11, LHKS12, LWWG12, LH14b, LH17, LZS+17, LMK16a, MRC+18, MLG18, MMH19, MSY19, MCF+18, MGCC19, MAK+14, Mat14, ME10, MKM+17, MFR+17, MMJ10, NS18, NF17, NN18, NO16, NFK+16, NFI+16, NS17, OHR18, ORZ11, OM12, OVPK15, PAK17, Piel14, Pil17, PW12, PZ15, QZ10b, RJBP12, RS13, Rez19, RB13b, RSG14, Rod13, RHPWS13, RHT+15, RSN19, RR19, REV+17, Rui11, RSKG14, SPS+12, SGPS+17, SH15, SS16a, SDF+17,
SFG$^{+17}$, SHL$^{+18}$, Sea10, SCW11, SDM$^{+16}$, SEF$^{+16}$, SE$^{+14}$, SH14, ST13, SHL$^{+13}$, SPR$^{+13}$, SZX13a, SZX13b, SMM15a, SMM15b, SMM$^{+18}$, SKTT11, SZSZ16, STS15, SK11, TLDg$^{+12}$, TN10, VGV$^{+11}$, density [VAR12, VECT12, VV14, Vik11, VI17a, VI17, VED10, VHS$^{+19}$, Vyb16, WKL10a, WHL$^{+10}$, WGL$^{+11}$, WCWW11, WWU12, WWCL15, WHX$^{+10}$, WL14, WTH$^{+16}$, XYW$^{+14}$, YLZ$^{+10}$, YS13, Yu12b, ZTH$^{+15}$, ZXS$^{+10}$, ZSWL12, ZKE$^{+17}$, ZDX11, ZLHH14, ZCWX18, ZGS$^{+10}$, dSdS12b, dSdLBNB17, dLC17, dLvNC18a, CDM10, FAS$^{+18}$, VV19]. density-based [LZS$^{+17}$]. density-density [DSAS19, SS16a]. density-fitting [Boz18, Hil13]. Density-Functional [YKNN19, Oht16, CHG$^{+16}$, HNW07, HNW12, IM17, JCP14, KZZ$^{+16}$, MFR$^{+17}$, NF17, NN18, NO16, NNK$^{+16}$, Rez19, RHPWS13, SPS$^{+12}$, VED10]. density-peaks [LZS$^{+17}$], deoxy [VM11]. deoxyribonucleoside [XVN17]. deoxyribonucleosides [RJWW12]. dependant [PNG10]. Dependence [CFM$^{+19}$, BRLS08, BRLS12, ELP19, FE14, GZZ12, KKO$^{+16}$, KGM12, Lar12, LPE$^{+10}$, LTLT12, MP17b, PZA15, PBE16, PS10, SGFJS$^{+17}$, SY16b, AD10, MGWR12]. Dependences [NNT$^{+19}$, SMM$^{+18}$]. dependency [DKT13, PHDH13]. Dependent [YKNN19, AALCM11, BS16a, CHG$^{+16}$, CP15, CP10, DP15, EPD$^{+10}$, GTK10, HNW07, HNW12, HG10, HYUS11, JYS$^{+12}$, KS18, KCPMG12, LPLS16, LZ12, LZGS11, Mat10, NS10, PAK17, PPJ14, PVJ10, RHPWS13, REL17, SY16a, SFBT17, Vik11, WHL$^{+10}$, WHX$^{+10}$, YLZ$^{+10}$, ZXS$^{+10}$, ZDX11]. depending [Lin18]. depolarized [KKK$^{+19}$]. deposition [SE14]. depth [DDP$^{+18}$], derivates [UGK18]. derivation [SCMA$^{+17}$, VVV$^{+15b}$]. derivative [MY17b, TPL$^{+10}$]. Derivatives [KTSW11, CWHH11, CZH12, CBTZ16, CROB16, GRN19, HSZ$^{+11}$, JS17a, JYS$^{+12}$, KG11, KPL15, LWGZ15, LWGZ12, MFR$^{+11}$, MIS$^{+15}$, NS10, NF18, PC14, RBV$^{+12}$, RFN15, REH13, SBR13, SZX13a, SZX13b, VVJ15, VYV18, VSD10, WGL$^{+11}$, WRP$^{+17}$, WDP$^{+12}$, ZsA10, ZWZ11, ZZ12, ZZWX11]. derive [RVP$^{+11}$]. derived [CIKT13, GMMH$^{+16}$, KSR$^{+16}$, LRVM18, LZGS11, MUGNVJ$^{+18}$, MCLD10, OSS10, PLZ17, REL17, SOYC12, SE14, TBSM12]. Deriving [CCYL11]. descent [MS16]. describe [LCK$^{+18}$, RHCHR16, RS13]. described [BM12, CCB15, KDS17]. Describing [MKGA10, CGA19, DAP$^{+18}$, JCP14, JBSQG11, MY17b, VBD11]. Description [FD16, MR17, Rez19, SWW$^{+19}$, BBG$^{+18a}$, BD12, BE16, Cam15, CRZ$^{+18}$, LAM19, LZLC13, MFR$^{+11}$, PM13, PLH16, PVAM16, RVM19, SRF$^{+17}$, SSA$^{+17}$, TKNN10, WvRSM14, WL14]. descriptor [DFP$^{+15}$, MA16, PRY1$^{+17}$, TMJ15, WMW$^{+10}$, Yap11]. descriptor-based [DFP$^{+15}$]. Descriptors [ELKE19, STF$^{+19}$, CBDS19, FCL$^{+10}$, FZL$^{+15}$, GJMPAM$^{+14}$, MdOdQ18, MCF$^{+18}$, MH10, NKJ16, PKIC11, RB13b, SIT18, TTB$^{+10}$, Wei12b, YLCX10, Yap11, YDX16, ZWX16]. Design [LI19, LLX$^{+19}$, LCM16, Spr18, SCSM19, Tak14, TZ12, VBD11, AM10, AFBR17, BAMR13, BEPM14, BPC13, CBP14, DPB$^{+12}$, DPOS16, DGL$^{+13}$, }
GS14, GMZ12, HSW+19, HHBY10, ISP+10, KSD+12, LABSG17, LBS10, MS16, NPG+18, PC11, SYDS11, SGM+13, Sti15, TKXT13, TRA+16, VVY17, VVMY18, VMV19, VMPS17, XHLH16, ZSB+11, ZWP11, ZYW+16, ZWS+10. designed [BL13]. Designing [PS+10, CSC+18, ZA15, Fe10].
desolvation [BK17a]. Desorption [UG18]. destabilization [XMA+19].
detailed [ABB+12, ABB+13, GPdC+16, KGJZ19, MP13, MO15, MC10].
details [MBA14, RSG+10]. Detect [RMRBH+19]. detected [TCP+14].
Detecting [DVVP14, HW19]. Detection [CBP+15, BV14, CLX+10, Man19a, ZLM+15]. detectors [SK13].

determinant [PM18b]. Determination [BP18, Cam19, KLS10, ABB+13, GPdC+16, KGJZ19, MP13, MO15, MC10].

DFT [BRLS12, CLFRO18, CPR18, SIG+15, YJ17, ZZY+16, AALCM11, AR10, AF14, ASMS10, BTMS12, BRLS08, BIL10, BTB+11, CLFRO18, CMM18, CCB15, CH10, cCVG+14, CBDS19, CXS10, DSB+19, DJD12, EFAC13, FVP14, FPR14, GNASBF16, GRN19, dCGR19, HDM+19, HSH15, HRJ+14, HRJ+15, HBI+17, HL19, JRSHP14, KG15, Kar17, KT12, KKL+13, KM13, KP10, LEDO1DV17, LBC+19, LRBB12, LZL+10, LZHH11, LZX+10, LSH+11, LYSS11, LZLC13, LH14a, LLSW14, LCM+14, MUN+19, MMS16, MPJ+19, MDTD16, MG15, Mat10, MS11, MVKS10, Mor15, MCK17a, MCK17b, NKLJ6, NC12, NMLD13, PTK11, PHK14, QLYL10, RS17a, RDF+11, RS14, RRC+15, RLZ+18, RN17, REL17, RKB+14, RK15, RRF+17, SWM10, SCF+19, SRL+15, SCMI19, SWW+19, SDL14, SZZ+18, SPZP18b, TNI+19a, TSNC+17, TG12b, Tsi14, TS15b, Tsi17, VVJ15].

LMI+14, PG18, PVS12, RS13, SZZS16, VT14, VMV19, YJ19, Zha11, dSH19.
Dimetallic [ZYG+14]. dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18]. dimethylaminoazobenzene [KP10].
dimethylaminophenyl [YLZ+10]. dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
edited [IN13].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
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dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
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dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
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dimethyl [GC11, KPH+19, WLC12, ZSWL12].
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dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
dimyristoylphosphatidylcholine [ML14].
Dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminophenyl [YLZ+10].
dimethylaminosilane [FFA14].
distribution [Bou14, COHI19, HDK+12, HNS16, JLCA17, KS18, MLG18, SK18, SYH12, TKN10, YKO+11]. distributions [AS15b, BCSCJ+13, GWF11, GMG+10, LRER13]. disulfide [ZYS+10].

[CSXZ17, SZX13a, SZX13b, ZWLX11, ZWX19]. **Douglas** [YS13]. **DOX** [RCR+16]. **DPO** [WGL+11]. **DPPC** [LBDP12, vRWGS17]. **DPT** [BH13, BZI14]. **Dramatic** [MLY+13]. dramatically [CSC+18]. **Draw** [LBB+15]. **drawback** [BRGN12]. **Driven** [IPAA11]. **Driving** [YZLZ18, RN17, YZ17]. **Droplet** [SJSS19]. **Drude** [ALRM18, LRvdSM15, LM18a, Ric16, SM14b, ZM10, HLEM18]. **Drug** [GSHM10, MBA14, AJA+19, FLM11, GMASBF16, HSW+19, Ibr11, ISP+10, PC11, PVJ10, SZZ+18, VHA+10, Won18]. drug-like [VHA+10]. **druggability** [LG14]. **drugs** [PPUBGD10]. **DSCs** [YJN+11]. **DSiCl** [LX11]. **DSPMP** [FZL+15]. **DsRed.M1** [SGDT10]. **DSS** [GZM11]. **DSSCs** [ZSTRS+18]. **DTTO** [MCAG+16]. **dual** [JCG+10, MA16, TMJ15]. **Duncanson** [Bac12]. **duplex** [HDK+12]. **Durandal** [BSZ+12]. **during** [GBPCC19, GNDA+12, LBC+12, MJLV14a, MJLV14b, OSA19, PNG10, RSKG14, dCDP15]. **dyad** [KP10]. **dyads** [KCK+15]. **Dye** [MP19a, ACS12, JYS+12, SLZ+15a, SLP+12]. dy-aggregates [ACS12, JYS+12, LCLZ+15a, MP19a, YJN+11]. **dyne-sensitized** [YJN+11]. **Dyes** [FAS+18, DBM+17, NPG+18, VAA+14, WJG+13, YJN+11, ZSTRS+18]. dyne* [FA18]. Dynamic [LKL10, SFA17, SZB19, VSP19, TNYN16, AKK+16, BS10a, BMB13, CVT+11, ESM+12, GBL+11, Hel13, MB14, NNY+17, OPR16, VOR12, WFS19, PBDW11]. dynamical [ALH+10, EFOD13, Ham11, VVMY18, VPR10]. dynamically [HS17a]. **Dynamics** [AIM+18, BHF+18, BHB19, CPV+12, LK13, MFEM16, NNT+19, NN19, AASP18, AJA+19, AALCM11, AG11, AS15a, Aki16, ASL+11, AB11, APK14, AB16a, ALH+10, BHB12, SBL11, BDDTP11, BJSI12, BW15, BF17, BMBJ11, Bow16, BEL+11, CTR13, CSl+14, CH16, CCOH14, CCW+10, CHK10, DASA15, DGA+11, DNN15, DSD+11, DTZT+11, DJS+18, DLZ15, DMT+15, DL19, EP10, EK15, EPH+13, ETLS17, EFOD13, EvRC+18, Fon13, FBEM11, FPH+19, GBL+11, GDV17, GR11, GKB+19, GWZ15, GCW14, GGM+12, GPdC+16, GP11b, GC11, HZ11, HS17b, HKNH18, HHHK19, HCD+10, HP10b, HPT17, HPSK12, HJ10, HHWL17, HLEM18, HRID16, HC14, IUK+11, ISK14, IN19, IM17, II10, IPAA11, JIS13, JA10, JSBSQ11, JCG+10, JAH+17, JLS18, JWST10, JMS14, JS17b, JND+19, KT19, KCT+17, KCR+15, KVQ+11, KUDG12, KSNT19]. **dynamics** [KGHC15, KCC+18, KDB13, KB14a, KNE11a, KERY+16, KLOS+17, KMG+17, Kop19b, KSR+16, KG13, KZP+18a, KN18, KV15a, KVR10, LLI15, Lar12, LWK+14, LH11, LJR+12, LL13a, LRvdSM15, LCH10, LHC+13, LLI+14, LPE+10, LLTC12, LZS+17, LPLB16, LL12, LBPD12, MBT+14, MMH19, MSY19, Man19b, MKS+12, MSC+10, MJ14, MN15, MCRL17, MLN+18, MFEM15, MADWB11, MKM+17, MB16, MHR11, MO17, MO17, MIOM13, NPTS16, NST14, NFPD13, NFG+13, NNN+16, NHK+13, NTNY15, Oht16, ON14, OGL10, OCL11, OLY17, OT12, OCW+15, PMC+17, PSS14, PAK15, PH17, PP19, PL14, PM13, PD12, PHT17, PVZ13, PS10,
PVAM16, RD18, RS12, Ras17, RO14a, RO14b, RFN15, RR14, RdA12, RVdMB16, RC18, RLG14, REL+14, RSR15, RSB+13, SHMO11, SF18, SLT+15, SKA19, SWM10, SSWX14, SS19, SSNT19, SOM+13, SCK18] dynamics
[SIJ17, SR18, SYN+12, SM16b, SK13, SKMS13, SFLG+17, SLLL13, SI16, SZZ+18, SV11, SPZP19, SBvG14, SAVG15, Tac9, Tac17, TNYN16, TFYO19, TJR19, TTC+18, US11, UGK18, Vor10, VM11, WKLC12, WBN+13, WAM17, WC11, WHL+10, WH11, WWKS11, WLC12, WLF19, WES13, WG14, Won18, Wu10, WBE16, XCLZ19, YPvD13, YO19, YHX19, YJXZ13, Yon16, Yu12a, YFH+19, ZZY+16, ZX11, ZDKM12, ZBP11, ZP13, dCLFGL13, dSVdM+16].

Dynamics-Based [AIM+18, Vor10]. DynamO [BSL11]. dysprosium [BP18].


Effective [GKV+13, IM17, YZ16, AASP18, CVG14, DR11, DMN14, DMN15, GA12, HKNH18, KS13a, KS15, LCM+14, PHC13, PRY+17, PS13, RLD12, SSB+16, UCFR16, WXS+12, YZZ16, YZ15b, ZKH+10]. Effects [CS14, GBG+19, HTY19, JAH+17, JLLW19, LGOM+15, LCH+15, Mor15, NNT+19, SEM12, Tac17, WWTL19, YCK16, dCRN18, AS15a, ATIP18, AS18, AK10, ASK18, BBI+11, DMD+18, EPH+13, FAA15, FD16, GNC+18, GMG+10, HS16b, HDM+19, HLBCCG15, INT18, IN19, JMX+16, KIOY19, KG11, KYCL11, KHE+19, KKA+18, LGVA14, LHT15, LWD13, LKZM18, MUN+19, MKGA10, MBC11, MRK11, MLY+13, MUC15, MGS+16, MKK+19, NASH15, ORZ11, OSHG17, OCW+15, PLFS18, PMT10, PP19, PC14, RMGB11, RRK16, SSWX14, SMP17a, SFLG+17, TM16, TYN15, TY10, UT14, VP19, VKAM12, WXY14, YNH+17, YJ11, ZZP+16, Zha11, ALW+10, TIP+15]. Efficacy [LC17a]. efficiencies [RO14a]. Efficiency [AC11b, BB11b, BB11c, FE14, GBSE11, XFG+16, AC12, FSSW19, GSHM10,
Eigensolver [KZZ+16, KCC+18].
eigensolvers [ZVY+15].
eigenvalue [Coh18, HLXH17, HLXH18].
eight [HDK+12].
either [TCPPC14].
elastic [ECZWD17, LBTV11, QB10, QB11, SH11a, XTY+14].
Electric [GH16b, LL13b, BLFZ13, BLBG+13, BS10a, CXXS10, GH16a, KMT+19, KZK+12, MRB14, PDC18, SH15, SLX+15, YL11, YJ11, YCK16, ZSL17, ZX19].
electrical [LLL11].
electro [TMJ15].
electro/nucleophilicity [TMJ15].
electrochemical [SKGP19, SIG+11, SGH+16, YJ11].
electrochemistry [DSK17].
electrode [IN19, MKO+13].
electrodynamics [Tac19].
electrolyte [KS18].
electrolytes [HAL14].
electrolytic [SV11].
electromagnetic [SEM12].
electron [BK11, Bar14, BLG11, BWKW10a, BWKW10b, CEBO15, HS16a, HRMAL+13, HGCGGR+16, KGR+16, KKGW19, LLX+19, PII17, VSP19, VV19, WWU12, ACD+13a, ACD+13b, ABGD12, BH12, BT18, CDB10, CAA10, CW11a, CC18c, CJPTC18, CTP13, CXD+19, DA15, ED15, EP12, ESM+12, EP15, FRSA14, FWS+18, FED17, FCPJM14, GNDA+12, HSH15, HPT17, HEMCZE+14, HAP+12, HBL12, IYK11, Jan16, JBSQG11, JSF19, KPL13, KTK17, KKA+18, KYG+15, LW16, uLhY11, LRVM18, LH10, LYL16, LLJ12, LP11c, MRC+18, MKGA10, MRB14, MT19b, Mat14, MBFP15, MH+13, MCK17a, NYH+17, NLL19, NS17, PAK17, PGDO+16, PSC11, PS17, PNI13, PTB+15, PHT17, PC16, Ras17, Rod13, REL17, RSKG14, SFM+18, SZB19, SB14, SB17, SGL13, SK11, SSA+17, UCR18, VGV+11, VECT12, VL17a, VCL18].
electron [VI17, Vyb16, WL+10, WMY11, XBSS19, YKH+10, YL11, ZPP+16, ZCWX18, ZGR+10, dLC18a, dLvNC18a, GMBM18, SDIP18].
electron-correlation [NYH+17].
electron-deficient [YL11].
electron-hole [PTB+15].
electron-pair [WWU12].
electron-sharing [JSF19].
electron-vibrational [CJPTC18].
electron-withdrawing [CWHH11].
Electronegativity [FCPJ14, vS18].
Electronic [AMQ+14, AM19a, AM19b, ASS10, BAD+19, DSB+19, DAdGR15, DGSVGM19, GNDA+12, GNI18, HLWD15, Ibr17, JLL19, KYL11, KKL+13, KKGW19, LLBO12, LS11b, LKZM18, MT19b, MP19b, MAPB10,
NSN19, ND19, NIIT15, PMC+17, RLA+11, SZL19, TN12, TNI+19 a, TN10, TFQ+10, TS15b, VI17, WRM+12, YW12, ZRCC11, ZLX+19, AR15, AK10, AC12, BLZ+13, CPRS18, DKE+17, DHOG13, DMD+18, EVR18, EH13, EKW+13, EBPK17b, FB10, GTH10, GRARO+14, GWX+12, GZZ12, HASR+12, HS14a, HS+11, Hua16, IIF+10, KK1H19, KKPT11, KSM17, KG11, KKA+18, Kop15b, Kos16, KP10, LGOM+15, LX11, LBT1V1, LBT1V12, LNX+10, LSH+11, LLWS14, MC10, MA16, MCF10, MCF+18, Mat10, NC14, NCT18, NFI+16, OLA15, PiSC18, PHK14, PTB+15, PVAM16, Py13, RCM+13a, RML+15, RR12, RR11, SFA17, SLP+12].
electronic [SIT18, SB19, SRS14, ŠB15, SKGB13, Tac19, TFQ+11, TD10, TS15a, TNG+10, TS11, TG12b, Tsu19, TEDT18, VVP12, VHR16, VAR12, VBMA13, VLKG+17, VGT116, WHL+10, WGL12, WJC+13, WO15, WSGN11, WZK+13, YK13, YFH+19, ZJZ13, wZhZ11, ZBB16, ZZZ+19, dCDP15, dVAG16, vSGP10].
Electronically [SCSM19, BSL+16, LSH+11, LYSS11, RIJ+11, SFCCK+14, SFCCK+15, YB11].
electronics [Sah18, EKH14, FHZA+18, WCY+11, WRG+17, XhD15, YCGA10, SGP18].
electrophilic [MA16, WDS+19].
electrophilicity [YB16].
Electrostatic [CLA16, LP11b, MLZZ12, Sch18, VSP19, WFZ+18, ALRM18, AS18, BT18, BCNH+11, BSF18, BK13, CCC+11, CS14, CPK12, CB11c, DLSA14, ER18, GBL+11, HOK17, IO13a, KTN10, KYG+15, Lar11, LCA17, LCM16, Mat14, NF18, OHPR18, PV110, RB13b, TY10, VMMR+17, VVY18, YKO+11, YWJ+16, YAO18, YMP14, YZL+15, ZDM13, ZBP11, KGM12].
Electrostatics [BSG18a, CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NLP+16, SDZ17, SWPR11, UHH+11, XYX17, YMP14].
element [BCCO10, GPK+16, RMGB11, TG12b, TCX+13, XYX17].
elementary [LPLB16, Zim13].
Elements [TKN13, BV14, CWZB10, Hil13, JJ16, LF14, SK15a, TDKT10, Ts14, WSI2, XhD15, MSCP19].
elevation [HH10].
ELF [RSKG14].
ELI [BWKW10a, BWKW10b].
ELIA [BWKW10a, BWKW10b].
Eliminating [vS18].
elimination [SL10, dCDP15].
Elisabeth [Hil12].
ellipsoidal [DBG+13, LDG+15].
Elongation [OLA15, MKGA10, MKGA10].
Elongation-MP2 [MKGA10].
Elucidating [HNHR13, TDP+12].
Elucidation [CPLL11, TNY16].
embedded [DS17, GMG+10, HSH15, KMT+19, ZFS18].
embedding [CCB15, ESD18, ESM+12, HH16a, HH17, Höf14, HOK17, KSR17, NF18, NOKJ16, RR12, SDF+17, SS16b].
Embelin [CPR18].
emerges [MNNK10a].
emission [CSC+18, LX11, MCLD10, PLP+16, SGWA17, WDP+12, ZLL+10].
emitted [PE11].
emitters [FWS+18, ZGZ19].
emitting [FWS+18, ZGZ19].
Emphasis [RCM+13b, PD11].
Empirical [BA11, DLMH12, KLN12, CK17, DAG19, KB10, LL11, MPBJ11, PTK11, RJPB12, SZBM13, SBvG14, TM16, ZRL+15, ZM10].
empirically [VCL18].
employing [GP11b, MLCD11, TG12b].
empowered [BPLL12, RLLHL12].
enabled [Aou16, BK17c, KYG+15, LL10a, SR11].
enables [KK17a, RC18, XHLH16].
Enabling [PHH+12].
enamine [AS11].
Enantioselective [ORZ11]. enantioselectivity [OAN15b]. encapsulated [EOO+16, STS15]. encapsulating [WZH+18]. encapsulation [YDGZ15]. encoded [RSL16]. encoder [LDH+14]. end [HDL+17, SL10]. ended [RJR14, Zin15]. en. [FB14a]. Endohedral [NKD18, FL15, MCK17a, MCK17b, ZSL+11, ZYG+14]. endohedrally [DK11, ELKE19, AF14, AS14, AG12, ABS+19, BW11a, BLF14, BVH17, BS16b, BE16, BS18, CHG+16, CMD13, CR19, CH10, CTP13, CXD+19, CBG16, DHOG13, DMJ17, DHH+11, DPOS16, FGM11, GRN19, Gil11, GP11a, Gri13, HAGK10, HH10, HH11, HLW+17, HDM+19, HWWL17, IKN13, KSH13, Kar17, KSM17, KJDB12, KB11b, KYB13, LJW11a, LW11, LHLL14, LH14a, MCS11, MS13, Min18, MSÄK12, MBE16, MMJ10, NWW17, NMF+14, OBW12, yOTh16, OAN15a, ORS16, PGCT+12, PPJ14, RLDJ17, Ran19, RDDS10, RAR+11, RO14b, RZ16, RR14, Rob13, RJS17, SRR16, SK12, SHL+13, SOD+11, STM+15, SWA17, TS14, TSN16, UD12, VVG13, VECT12, VM11, WBT10, WS10, WJG+13, WSA19, WGA18, WG12, WX12, YAS13, YMP14, ZZ+14, dALdS15, dRBO13, NQB19]. Energy [DK11, ELKE19, GS16, IHY15, JCGVPHT17, Jia19, Kop19a, LFN+10, LPLB16, MYKO18, NK19, OSI+19, PK19, SN16b, SSGS15, Spr18, SKGB13, VL19, VSP19, WM12, ZQH19, AMGB10, AAB+19, AC11a, Ano10a, AK10, AK16, BCSJC+13, BPM15, BRE16, BH15, BS16a, BRLS08, BRLS12, BACSCJ+10, BG17, Bon14, Boz18, BD11, BWMSM10, BB11b, BB11c, BG12, CM13a, CK10, CDM+15, CLA16, CY09, CX0, CZY11, CY13, CH16, CSXZ17, Che17, CF18, CS17, CHR+12b, CHR+12a, COHI19, CKP10, CM+10, CPK12, CWZB10, DPG+11, DWR17, DBG11, DS12b, DH14, DWC17, EV14, FMNC11, Fer17, FED17, FCOCM12, FSSW17, FCP17, FLM11, GS14, GS15, GHK12, GO13, dCCCRN19, GMO16, HNYH19, HDM+17, HHNK19, Hei13, HDM+15, HH15, HG13, HYMZ16, HYUS11, HJKJ13, HGWI18, HYD10, HDHL15a, HDHL15b].
HNWF12, HH17, HZSS17, HDHL15a, HDHL15b, HDHL15c, JCGVPHT17, KT19, KPG18, KB14b, LLBO12, LLW12, LWGZ15, LGC19, LX11, LSH+11, LYSS11, MPSG11, MGCC19, MEH18, NYN17, PH10b, RRHCH16, RR14, SFCCK+14, SFCCK+15, SRF+17, SZZS16, TSN17, WHL+10, WHX+10, YD17, YHX19, YLZ+10, YB11, YYT12, LZL+10, PGW+17].

Excited-State [FHG+19, YKNN19, SGWA17, FD14, GA18, HH17, HZSS17, KT19, LWGZ15, MPSG11, NYN17, PH10b, WHL+10, WHX+10, YD17, YHX19, YLZ+10, YB11, YYT12, LZL+10].

excited-states [LLBO12]. exciton [HRH+17, LSH+11, SEJ+18, WZ19, ZZL19]. exciton-phonon [WZ19].

EXcitonic [JCGM18, NNT+19, LCK+18, ZMMM12]. excluded [LWZ+17, Yan14]. exclusive [dLC18a]. Exhaustive [DKV18]. exhibited [RWR+13]. Existence [MBB13, WD10, NKK18]. existing [KT18].


expensive [LDZW17]. Experimental [Cam19, MRC+18, NHE+10, AvKSP16, BRGN12, DCDOD13, EOO+16, GPSC+16, HJ13, KIP10, PO14a, SB10, SGS+16, SKMS13, VZ14, CVC+10].

expected [LZGS11]. experiments [CBP14, HCBI].

Explicit [WG14, BEM14, CCH14, CBG16, EK15, ENKK+17, GLB16, HDL+17, KJDB12, LH11, RdA12, SYH12, SKMS13, Zha12b]. Explicitly [yOT+16, SM17].

Exploiting [HB14, BYE+16]. Exploration [FHG+19, OSI+19, ZGS+10, BGL+18, CF18, IWW12, LAW+16, NJR18, OKIS17, OKY18, RDRC16, Sti15, SPP+19b].

explore [JCPC11, MNB+10, MCC12].

Exploring [BHB12, BPPS17, BPS19, BCG10, DSHLM18, ELKE19, FDH19, MTM14, PJ13, Ts17, VHS+19, ZT14, sDsLBNN17, RDRC16, NOKJ16].

explosion [GC18]. explosive [YPC+10]. Exponential [BB11b].

expressions [Gav12]. extended [GWZX12, IN19, KUDG12, LRvdSM15, SSWX14, TSN17, YB16, PON11].

Extending [LMZ11a, Man13, TTN19, VB13a, VB13, PHH+12].

extensible [GCW14, JYC+16, LAS+14]. Extension [AlQ19, HSN14, PFVL14, SDZ17, VW+18, YHVM12, Cam15, LL11, RRLHL12, Ras17].

extensions [NYH+17].

Extensive [JW12, SLHW09, YB11, CF14, KM13].

Extent [OSA19, FGS18]. exterior [HL19]. exterior/interior [HL19].

external [GKSS14, KMT+19, PdSC18, SEM12, XTN18, XMA+19, ZSLL17, ZX19].


Extreme [HRH17, Cam15, DS12a, JBSQG11, CCR18]. eXtreme-Pressure [CCR18].
Extremely [ZM11].

Kid19, KLJ+17, KSK11, KT10, KFT18, KGJZ19, KMLS10, KVR10, Lar1i, LvDH13, LC17b, LM18a, LPS+13, LPE+10, LN15, LLvG10, LvG13c, LL13b, LGD+15, LCL+18, MRO17, MBC11, MSS+13, MTvG12, MBE16, MLC13, MHR11, MP17b, NB19, NTNY15, ON14, PHC13, PLZ17, PdSC18, PG15, PZCL16, PLH16, PVM10, PS10, PNG10, Rod13, SH15, ST11, SM14b, SK17, SS19, SZBM13, Sie15, SYZ+17, SBvG14, Tak14, TYN15, VV+18, VHA+10, VPR10, Vik11, VVLG17, WXL17, WS19, WTH+16, WC14, WZK+13, WDHZ13, XP13, XVA+16, XMA+19, Yan11, YWZ14, YJXZ13, YJl1, YN15, YCK6, YHM12, ZSL17, ZL11, ZSYH12, ZVX19, ZDKM12, ZP13, ZM10, ZCGM11. field
[SYZ+17, SBvG14, Tak14, TYN15, VV+18, VHA+10, VPR10, Vik11, VVLG17, WXL17, WS19, WTH+16, WC14, WZK+13, WDHZ13, XP13, XVA+16, XMA+19, Yan11, YWZ14, YJXZ13, YJl1, YN15, YCK6, YHM12, ZSL17, ZL11, ZSYH12, ZVX19, ZDKM12, ZP13, ZM10, ZCGM11]. field-based [HKR12]. field-dependant [PNG10]. field-dependent [DP15].

Fields [Coo19, AS15b, BHI19, BVY+12, BAS14, CCLP12, CPN+17, GCWS15, GMMH+16, HDPM14, HJ10, JYC+16, KT18, KWL+16, LZZ+11, LZS11, LGL11, LTP11, LBDP12, MSK+10, MSK+12, MS15, ST11, S Gly+18, SEM12, TTC+18, VV+15b, VHA+10, WKC+10b, WLC12, WGI2, YPKB12, ZRL+15]. fifth [KM13, LOB18]. fifth-rung [KM13]. fifth-rung [DP15].


First- [TKNI3]. first-order [BCCO10, SK12]. First-principle [CCJC10, DBM+15, LLB+12]. First-Principles [HFSO12, BE12, BE14, EB12, EBK13, EBPK17a, JCG+11, LLLM11, wZbZ11, BPE16, EMD17, EB18, GD10, KLZ+18, PLZ17, RZG+13, WY+15, WD10, ZWMW10, Z12, vADC+14, HYL+11, SPZP18a].


fluorene [CH10, HXM+16, PH10b, YJN+11]. fluorene-phenylene [CH10].

fluorescence [CH10, EJ13, FWS+18, LM18b, VM19, ZLL+10, ZGZ19]. fluorescent [CSC+18, LZL+10, NSO+14, PGW+17, SCF+19, WJG+13].

fluoride [LCC18, LZL+10, MBRC16, NC12, RAB12, SBGP18, SRL+15].

fluorides [ASS+17, Sán17]. fluorinated [DK17].

fluorine [VMV19].

fluorine-centered [VMV19]. fluorobenzene [KS13].

fluoroquinolones [MPNS13].

fluorene [CH10, HXM+16, PH10b, YJN+11]. fluorene-phenylene [CH10].

fluorescence [CH10, EJ13, FWS+18, LM18b, VM19, ZLL+10, ZGZ19]. fluorescent [CSC+18, LZL+10, NSO+14, PGW+17, SCF+19, WJG+13].

fluoride [LCC18, LZL+10, MBRC16, NC12, RAB12, SBGP18, SRL+15].

fluorides [ASS+17, Sán17]. fluorinated [DK17].

fluorine [VMV19].

fluorine-centered [VMV19]. fluorobenzene [KS13].

fluoroquinolones [MPNS13].

fluorene [CH10, HXM+16, PH10b, YJN+11]. fluorene-phenylene [CH10].

fluorescence [CH10, EJ13, FWS+18, LM18b, VM19, ZLL+10, ZGZ19]. fluorescent [CSC+18, LZL+10, NSO+14, PGW+17, SCF+19, WJG+13].

fluoride [LCC18, LZL+10, MBRC16, NC12, RAB12, SBGP18, SRL+15].

fluorides [ASS+17, Sán17]. fluorinated [DK17].

fluorine [VMV19].

fluorine-centered [VMV19]. fluorobenzene [KS13].

fluoroquinolones [MPNS13].

fluorene [CH10, HXM+16, PH10b, YJN+11]. fluorene-phenylene [CH10].

fluorescence [CH10, EJ13, FWS+18, LM18b, VM19, ZLL+10, ZGZ19]. fluorescent [CSC+18, LZL+10, NSO+14, PGW+17, SCF+19, WJG+13].

fluoride [LCC18, LZL+10, MBRC16, NC12, RAB12, SBGP18, SRL+15].

fluorides [ASS+17, Sán17]. fluorinated [DK17].

fluorine [VMV19].

fluorine-centered [VMV19]. fluorobenzene [KS13].

fluoroquinolones [MPNS13].
KLN12, LCW12, LBGS16, LGW12, LBTV11, LBTV12, LHKS12, LH14b, LH17, LPM17, MMH19, MSY19, MAK+14, MJW+11, MAP18, MFR+17, Mor15, MMJ10, NS18, NF17, NN18, NO16, NNK+16, Oht16, ORZ11, OMI12, PAK17, PPH+14, Pic14, PD11, QZ10b, RJPB12, RS13, Rez19, RB12.

functional [RSLML12, RHPWS13, RHT+15, RNS19, RR19, Rui11, SPS+12, SH15, SFG+17, SHL+18, SCW11, SBT17, SEF+16, SE14, SH14, ST13, SHL+13, SPH11, SH19a, SMM15a, SMM15b, SMM+18, SKTT11, SZZS16, STS15, TLDG+12, TG12a, TS10b, UvSvdWK19, VV14, Vik11, VL17a, VI17, VLGK+17, VED10, VKC10a, WHL+10, WCWW11, WDLG12, WYT17, WXH+10, WL14, WTH+16, WGN+16, WZC+19, YY+14, YJ11, YLZ+10, YS13, ZXS+10, ZWLX12, ZLZ14, ZYG+14, ZYW+10b, ZYW+10a, ZLHH14, ZGS+10, dSDS12a, dSDS12b, CKH19].

functional/basis [PD11]. Functionalities [LJC+19, KAG+12].

functionalization [WWTL19]. functionalized [KYKR15, LdSRR16, LTR18, MSY19]. functionals [Ben17, CCB15, CGR16, CXD+19, DH17, DOM+11, DWC17, ELF19, FPRS14, GWRJ18, HG10, HBI+17, KB10, KSH13, KSSH13, Kar17, KM13, LBH+11, LAM19, LH14a, LK16a, PW12, RSG14, Rui11, SGPJS+17, Sea10, SDM+16, SH18a, SPR+13, SZX13a, SZX13b, VCL18, WYT17, Yu12b, ZTH15, ZWX19, dSDS12a, dSDS12b, CKH19].


[RSR⁺12, OYK⁺11, Bou14, CGA19, DLL⁺10, EPD⁺10, FRC18, IT19, JLCA17, LOB18, Leh15, MG11, MKB⁺13, OLPB19, POB13, SFI11, SH19a, Sun15, TH13, VKTRMJ15, ZKE⁺17]. Gaussian-based [CGA19, JLCA17].


**GC-related** [GX⁺12]. GDP [SS13c]. Ge [Cas14, MCK17b, PMG⁺16, Sak18, UT15, YW12, YLY16, WKC11].

**GeauxDock** [DFF⁺15]. GeC [HSY⁺11, Kop18]. **GeH** [Kop19b].

**gelatinases** [XDL⁺10]. Gelessus [Spr10]. gene [CQFC10]. **general** [AA18, BSL11, EWK⁺13, FNSF⁺11, HSN14, Ish12, NLP⁺16, PH17, RJR14, Sun15, VHA⁺10, YHVM12]. general-contraction [HSN14].

**Generalization** [Sah18]. Generalized [GH16b, KCPMG12, MSPC19, AB16b, BSPP⁺13, DSF17, FCE15, GH16a, HWL11, LL10a, MA16, NMH19, PS13, SZTSM10, SSB14, VMPS17, WWKS11, WHM10, WBVE16].


giberellin [HYYZ13]. giberellin-binding [HYYZ13]. Gini [WF16].

**GIPAW** [SPZP18b, SPZP19]. **GIST** [RNSF⁺16]. give [AA18, JT18]. glass [GFSG18]. glasses [You10]. 

**Global** [LvDH13, OKIS17, PRSG13, Tak10, VL19, BK17b, CPN⁺17, CZZL19, DS15, DMAH15, FDH19, GPE13, LK11, LL11, MP13, MB14, MO15, MCA1Y15, SKKS13, SC15, TSZQ12, Vor10, WDHZ13, XhD15, XCLZ19, ZL11, DH11].

**Glu** [JL13]. glucopyranose [HH10]. glucosamine [ZBP11, ZP13]. Glucose [APY⁺16, WFL⁺19]. **GLYCAM06** [SA10]. **GLYCAM06/TIP3P** [SA10]. 

**Glycan** [JSD⁺11]. glycine [DB12, DP15, FCD10, MC10, SPZP18a, SPZP18b]. glycoconjugate
[LABSG17], glycol [MSY19, TFYO19]. glycoproteins [JSD+11, PFVL14],
glycosaminoglycan [CHKR10, SZdB19, SA10]. glycosidic [HH11].
glycosyltransferase [RN17]. Gmbh [Spr10]. GMCT [UU12].
Gneimosim [LWK+14]. gold
[Ano15-58, BH14, CCJC10, FHT+15, FDH19, GAMAC+14, Li14a, Li14b,
LHKS12, LH14b, MFR+11, MG14, MBFG15, SRR16, SKTT11, YLL11].
gold-thiolates [FHT+15]. Goldberg [WTH+16]. Good [SB10]. GPCR
[LLHM16, MFR+117]. GPGPU [UM13]. GPR119 [HK18].
GPGSM11, GPGSM12, Ihl12, MCC12, PsdPE+10, Pog10,
RPNP10, dLvnCl8a]. graph-based [DH14]. Graph-theoretical
[WSH10, PsdPE+10, Pog10]. graphene [YZZ+17]. graphene
[BSD18, CMM18, dRcFGRB18, DJX+11b, DJX+11a, JWO15, KMT+19,
Lin18, LWZK13, LCM+14, PL18, RRK14, RLZ+18, SDF12, WCT+11,
WSZW15, WYL+15, WTH+16, YSSB12, YZZ+17]. graphic [HASR+12].
Graphical [SJL18, All11, GBL+11, HZY+10, HSW+19, LLLC11, LBB+15,
PVZ13, SEF+16, STH+10, WSGN11, WS13, YWJ+16, YDL+10, YN15,
YS10, ZKE+17]. graphics [AB16a, AB16b, BDTP11, CKKK16, EP10,
HKK12, HEMCZE+14, MSSP17, SR11]. graphite [Fom13, IN19, LAM19].
graphitic [LL13b]. graphs [AGR11b, RNPI3, RNVPI3, SOJ14]. Gratzel
[VAA14], gravitational [DS15]. Grcarma [KG13]. green
[LWL+11, NSF+14, PGW+17, yOTn16]. greener [ZX19]. Gregori [Hl12].
Gregori-Puigjané [Hl12]. Grid
[BAMR13, CPK19, HEMCZE+14, BPLL12, CGA19, CKKK16, FHMB15,
KP11, KKH18, LZ11, LLZA12, MMM+16, NCT18, RLLH12, dVZ17, CM13b].
Grid-Based [CPK19, BAMR13, HEMCZE+14, CGA19, KP11, KKH18,
LZ11, LLZA12, MMM+16]. grids [DH17, Min18]. Gro2mat [DDK14].
gromacs [Nav18, AG11, Abr11, Gar12, GP11b, KPF+15, KPF+19,
Hierarchical

High

High-Performance

high-resolution

high-temperature

higher-dimensional

high-throughput

higher-order

high-confidence

high-accuracy

highlighting

Hirshfeld-based

Hirshfeld

histidine

homodesmotic

homoarginine-containing

homoarginine

homologated

homology

horizontal

hormone-dependent
hormone-receptor [OME16]. horsetail [MCRL17]. Host
[CC18b, OA15b, YDGZ15]. hot [HQSZ19, RFHG10]. Hou [JW12]. HOX
[dSDdAR10]. HRPA [SPHF18]. HS [XCLZ19]. HSE [VLZK17]. HSiCl
[LX11]. HSICl/DSiCl [LX11]. Hua [JW12]. Huang [MT19b]. H¨uckel
[FL15, SKTT11]. Huffman [QLQ11]. Huge [NN19, NNK16, OHPR17].
Huge-System [NN19]. huisgen [ZZWT12]. human
[JAHS19, OME16, SLY10, ZX11]. hunter [CMF17, She12]. Huzinaga
[Fer13b]. HXeOXeF [ARLP13]. HXeOXeH [ARLP13]. Hybrid
[CGR16, KS15, NS18, VVY17, ZDKM12, BTA13, BG13, CBG17,
CSKH15, CSXZ17, CC11, DR11, DJ13, EL19, FHT15, GRN19, GFG11,
HZSS17, JAHS19, JMS14, KN17, KKR13, KJM17, LBH11, LT14,
MIS15, OK16, PW12, RSG14, SGPS17, Sea10, SH18a, SZX13a, SZX13b,
VCL18, VN17, ZWLX11, ZWL13, ZWX19, HPT17]. hybrid-meta
[BG13]. hybrid-parallel [KJM17]. hybridized [DC13]. Hybridizing
[RDRC16, FZL15]. Hybrids [VL19, KM13]. hydratase
[LT13]. Hydrated
[ALH10, BMFG16, CGP11, GBL11, NGCA10, LPE10, LBPD12,
VPR10]. hydrates [LZLC13]. Hydration
[BSC18b, HL14, AS14, DQ16, KB11b, KY13, OK16, PP10, RZ16, SK12,
SC18a, SWPR11, WBT10, WC13, WG12]. hydrazine [GZL12]. hydrazo
[WDLG12]. hydrazo-1 [WDLG12]. hydrazo-H [HPT16a, ZZWT12].
Hydride
[Jab18b, PM13, RKDM14]. Hydride-Triol [Jab18b]. hydrides
[DM15, PG12, RMGB11, WKC11]. hydric [Jab14]. hydroamination
[KT12]. hydroazidation [YXZZ17]. hydroboration [ZX19]. hydrobromic
[CY17]. hydrocarbon
[CB11d, IT19, KSM16, Kar17, MI17, SV15, WD12]. Hydrocarbons
[JCHT18, FVB10, NMI19, PL18, Ran19, SBvG14, ZWX19].
hydrocyanation [HDB15]. hydrodynamic [AKK16]. hydroformylation
[BF19b, dSDdAR10]. Hydrogen
[AFSW16, EHT19, ELKE19, EV14, HvM17, JLIW19, JT18, KKK19, MYT18, PNE18, PZM15, TD11, TL16, WKC10a,
WLH12, WFZ18, YZL15, AAMD11, ASK18, BEM14, BEMP14,
BLFZ13, BK17a, BLDK13, CK10, CSAdOM17, CPV12, CD11, CSXZ17,
CKP10, DKT13, DLT17, DBG11, DL19, EHSPT16, GNC18, GGM12,
GY12, GC11, HW19, HvM16, JCP14, JCG10, JSW10, KTT16, KSNT19,
KNP12, KGJZ19, LC10, LZH11, LJIW11a, LZJ11, LLW12, LHHW14,
LCC18, LTP11, LYSS11, LZY12b, LAW16, MPSG11, MK13b, MKO13,
MS11, MB14, NHF10, OKK11, PG12, PG19, PAT10, PD11, PNT16,
QZM11, SZ17, SSGS15, SKGB13, Tan19, TDT19, UT15, VVP12, VVY17,
VECT12, VDVR14, WLKC12, WHL10, XMA19, YR13, YLZ10, YI17,
ZDX11, ZLY16, ZW17, dCRN18, vADC14, SK13, SMD18]. Hydrogen-
[WFZ18]. hydrogen-abstraction [GY12]. Hydrogen-bond
[TD11, BK17a, CD11]. hydrogen-bonded
[BLFZ13, DKT13, JCP14, LJW11a, LHHW14, PAT10, UT15, ZDX11].
hydrogen-bonding [LCC18, PD11, WHL10]. hydrogen-bonds [LZH11].
hydrogen-bridged [ZLY+16]. hydrogen-contaminated [YR13].
Hydrogen-Disordered [MYT18]. hydrogen-storage [BEM14].
hydrogen-transfer [ZW17]. hydrogenase [GS11]. hydrogenated
[MRC16, wZbZ11]. Hydrogenation [GBG+19, JAB16]. hydrolase
[BHNS14, LD18]. hydrolysates [LWZ+19]. hydrolyses [YZGS14a].
Hydrolysis [JAHS+19, LHT15, MFM+12, XZ11, YZGS14a]. hydroperoxyl
[AAEM+11]. hydrophilic [PAK15].
hydrophobic [ARRC15, GMMH+16, JGS+17, MB11, PAK15, SY16b, TM16].
hydrophobic/hydrophilic [PAK15]. hydrophobicity [CH14, SV15].
hydroquinone [PNE18]. hydrosilylation [DK19, SSD19].
hydrostatic [FCW+14]. hydroxamate [GWZ15, GPdC+16].
hydroxamate-containing [GPdC16]. hydroxy [FFA14].
hydroxyapatite [XYW+14]. hydroxybutyrate [SJD14].
hydroxycoumarin [LZHH11]. Hydroxyl
[BHP19, DPNM11, GKR13, KS13b, Ray13, RKG11, SY16b, TM16].
hydroxylation [TLY+12, VCM15]. hydroxylations [MRR11].
hydroxymethyl [HH11]. hydroxymethylfurfural [APY+16, WFL+19].
hydroxynaphthaldehyde [MPSG11]. hydroxyphenylpyruvate [DGH+11].
hydroxyquinolin [CSC18]. hydroxyapatic [XYW+14].
hydroxylation [TLY+12, VCM15]. hydroxylations [MRR11].
62
dCGCRN19, HPT17, HRJ+ 14, HWLW11, HHWL17, KTT16, KT12, KTNN10,
KMLS10, MBC11, PPUBGD10, SOD+ 11, Tsi19, WH11, YK13, ZSYH12].
II/III [dCGCRN19]. III
[BP18, IKN13, KPL15, LWL+ 11, LXZ+ 10, SRL+ 15, BEL+ 11, CWT+ 12,
DSHLM18, GZZM16, dCGCRN19, HIS17, SKA19, Zha12b, ZKH+ 10]. III/II
[KPL15]. IKP [HLS12]. Illuminating [NSO+ 14]. illustrating [RML+ 15].
illustration [RP15]. im [FHG+ 19]. Image
[Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h,
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Ano15b, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o]. Image
[Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15y, Ano15z,
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Ano15d, Ano15e, Ano15f, Ano15g, Ano15h, Ano16a, Ano16b, Ano16i, Ano16j,
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Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17z, Ano17-27,


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information [CDS16, CCYL11, DWL11, GBVA11, ISN13, RSL16, ZLW10].

inspection [KOY+12]. inspired [CYY+17, DSM+11]. instability [MMH19]. instantaneous [RO14a]. Instanton [MK17, MK19, MRK11]. Insubria [GCC14]. Insulator [LLL+12]. Insulin [MV17]. INT [YJXZ13]. INT-DBD [YJXZ13]. Integral [Coo19, VSP19, DL19, KSNT19, MEH18, RFN15, SS13b, Sun15, VKAM12, WXY14, YS18]. integrals [CHC+13, PS17, PC16, RLA18, SZTSM10, WDKT19]. integrase [XYL12]. Integrated [HSW+19, vRWGS17, CKKK16, MCC12, US11]. Integrating [APK14, LZZ14]. Integration [FPV13, AYYO17, BB11b, BB11c, DH17, LP11a, MOS18, NSK18, dRL11, Pol13, Pop18, SJ11, SJ16, dBO13, MYKO18]. integrative [ˇRez16]. integrator [JS17b]. intelligence [Aou16]. intelligent [CDS16]. intensity [dSH19]. Inter [CROB16, SSB11, I HY15, CKKK16, MCC12, US11]. Inter- [APK14, LZZ14]. inter-residue [HY15]. Interacting [CM16, VSP19, ATP18, EV14, HGCCGR+16, MP17a, PNE18, WL14, JCHT18]. Interaction [BHB19, CK10, CCCLCRO14, CCCLRRO14, Den12, NNS15, SBW12, YZWC11, ALW+10, AG12, BLFZ13, BLF14, BCNH+11, BSD18, BHB+17, BRLS08, BRLS12, BG17, CLFRO18, Cas13, CZH12, CYG+15, CTP13, CAP17, EK17, EV14, FF11, FCCP17, FA18, GA14, GP11a, HPT17, HBL12, HLH+12, HSZ+11, HLXH17, HLXH18, HQS19, HL19, JZZM14, Kan15, KTNN10, LL10a, LMZ11a, LPS+13, Li14a, Li14b, LHWW14, LZL+15b, LPLB16, LCWW10, Min18, MS12K12, MCP18, MVBD18, NGAS17, NN18, OHP17, OHP18, PRJ+17, RZG+13, RS13, SM16a, SS13a, SBGP18, SBV10, SHL+18, SPL+18, SHF11, SH19b, TYN15, Tan19, TSH+19, WSH10, WYL+15, YK13, YWJ+16, YAO18, YCK16, YHCS11, ZRC11, ZY14, ZW18, ZZZ+19, dLvNC18b, vS18, KCB12]. interaction-activation [LSL+19]. interaction-based [ZW18]. interaction-induced [BLFZ13]. Interactions [BGS+19, Hes19, Sch18, WCT+11, ZCK+16, Abr11, ARRC15, AKB+16, AO10, BSF18, BSDG18a, CSS17, C18b, CIKT13, cCVG+14, CKP10, CROB16, CB11a, CB11c, dRCGFRB18, DDP+18, DFP+11, DBG11, DLML12, EP10, ER18, GFP11, GZ15, H14, HSJ18, HLVdV13, HTY19, ICS+12, ICS+13, IHY15, Jab18a, KSSH13, KCK+15, KPH+19, KGJZ19, LZLC13, LZSM19, MLGB16, MH17, MKH+13, MR17, MJM+15, MVKS10, MG14, MF+17, MPBJ11, OHNK11, PPJ14, PLV+11, RTS+13, RVM19, RMRBH+19, SSIG15, SDF12, SB19, SWW+19, SSB11, SSB13, TNN17, TG12a, TY10, TSR+16, TNG+10, VV15, VM19, WS10, WGD+16, WDS+19, WZ19, WM17, XTY+14, XLY12, YKO+11, YZ15a, YW13, YZL+15, YDGZ15, YZLZ18, ZLL+12, Zha11, dLC17, dLvNC18b]. Interactive [BRP+12, BGR13]. interactivities [CQFC10]. interatomic [DPAB16, FCCP17, RLA18, YKO+11, dLC17]. intercalation [LAM19]. interconnections [GLF16]. interconversion [HH10]. interconversions [TCGNT18]. Interdependence [WAB17]. interest [BCNH+11, OZLSBH12]. Interface [SJJ18, AI11, BDTP11, CSSB11, GRP+12, GCW14, HL14, JJW+14, KG13, LJR+12, LZdL+10, LBB+15, MSSP17, NS18, OYK+11, PHH+12, PVZ13, RR14, RSR+12, SN16a, SYDS11, SISK10, STH+10,
ion-pairing [KTK17]. ion/water [SV11]. Ionic
[FDCJG18, JXSW15, APFI13, APY+16, CG15, CFC15, EK15, GC11, IN19,
IM17, LEDOLdV17, MG15, NFT+16, PS14, SCM+15, WWKS11]. ionicity
[SLY+19]. ionisation [CTP13]. Ionization
[SHL+18, ACD+13a, ACD+13b, BG17, CG15, CBG17, GWF11, HNyH19,
LGOM+15, LK13, yOTu16, SSB+16, SGHL13, Tac17, VL17a, VCL18].
ionizations [LGVA14]. Ionized [GMBM18]. Ions
[WFZ+18, AS14, BDTP11, CCL1R014, CC12a, EKH14, PRJ+17, PZA15,
SNS16, SGH+16, VHS+19, WKC10a, XP13]. IP [BK17b]. IP-tuned
[BK17b]. IPRO [PGL+15]. IQA [CSM16]. IR
[DCOD13, CWT+12, LWL+11, LXZ+10, WJX+10]. irGPU.proton.Net
[Kan15]. iridium [CWT+12, HDPM14, KB13]. Iridium-catalyzed [KB13].
iridium-containing [HDPM14]. Iron
[HS14a, AKMYB18, BH19, BG13, CTR13, DK19, GBGR16, HS+19, HS16b,
KPL13, KPL15, MC10, NH19, SBC+11, TS10b, VBMA13, EH13].
iron-containing [AKMYB18]. iron-porphyrin-carbonyl [BH19].
iron-sulfur [CTR13, HS+19, HS16b]. irradiation [WZC+19]. Irregular
[Sch10]. isocloso [LK16b]. isoconversional [DCS15]. isocyanide [TLY+12].
Isoelectronic [ZLX+19]. isoindolin [YZL18]. isoindolin- [YZL18].
Isolated [FL15, DS+19]. Isomeric [FL15]. isomerism
[dCGCRN19, RS17b]. Isomerization [BW11b, DBGO+17, EFB16, BLG10,
BMFG16, LL19a, MSBF16, OKIS17, SJ11, Su10, WCL+11, ZWZ11].
Isomers [CS16, ZWZ11, DSHLM18, Kar17, OKIS17, WCL+11].
isoselectivity [OSA19]. Isoster [EdOdS18]. Isothiirane [MM19]. isotope
[KT16, MRK11, NASH15, ORZ11, UT14, UT15, VKAM12, WXY14].
isotope-substituted [UT14]. isotopomers [UT14]. isotropic
[JK+16, Tak14]. isotropy [Tru18]. Issue
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Ano14-32, Ano14-33, Ano14-34, Ano14-35, Ano14-36, Ano14-37,
Ano14-38, Ano14-39, Ano14-40, Ano14-41,


Issues [GS16, MFEM16, XFG+16]. iteration [SBB10]. Iterative [Hei18, VV19, Gra15, HLXH17, HLXH18, HL19, SM18, TTN19, VHR16, ZVY+15, PGL+15]. iVI [CBDS19, EH13, KMS+19, MUN+19, MLGB16, MTS+19, VBMA13, WZH+18]. iVI [HLXH18, HLXH17, HL19]. iVI-TD-DFT [HL19].


KSM17, KKNN11, LCK+18, MSC+10, MCLD10, OSR16, PVL+13, PTK11, PML+12, PB14, VAMS14, WWD14, ZMM12. **Levels**

[Kop19a, AC12, BCSCJ+13, BY11, BACSCJ+10, HYD10, Hua16, KIOY19, KHWB17, Kop15a, Kop14a, Kop17a, Kop18, MK13b, dSaSL13], leveraged [EPH+15]. **Lewis** [EHSP16, KASH14, Lǎc14], LH1 [KPG18].

Li [AM19a, AM19b, DDM+15, JW12, RLA+11, YCGA10, YHCS11, BWKW10a, GNI18, RLA+11, TN12, YZLZ19, YCGA10, SBW12]. **Li-based** [GNI18]. Li/Na [YZLZ19]. Li/Na-ion [YZLZ19]. Libcint [Sun15].

LIBEFP [KS13a, KS15]. libKEDF [DWC17]. Libra [Aki16]. **Libraries** [LG11, RLL+10, WF16]. **Library**

[KSD+12, Ak16, DWC17, EKW+13, FRN15, KS13a, KS15, LrvE17, LMZ11a, LAS+14, MZZ11, RFN15, SC15, Sun15, VAR12, Yes12, Yes15, ZCWX18].


Ligand [DPOS16, KKH19, KC13a, LI19, MNNK10a, VKC10, ABD11, AG12, BKLA13, BPB11, BCG10, BBG+18b, BS10c, CMD13, CIKT13, CHR+12b, CHR+12a, DFF+15, FTW12, FBEM11, FRLN10, GHHK12, GDV17, GJK+19, GS11, GZ14, HKR12, HG13, IYT+19, KLJ+17, KL14, KYB13, KTO11, KTO13, L11, LLC+10, LL10b, L1W+11, LBS10, MC10, MGWR12, MG14, MFR+17, NST14, NR18, NFG+13, NMF+14, OBW12, OHNK11, OGL10, OSR16, OCLM14, OOT15, PGCT+12, PK17, PPI14, PLV+11, RLD17, RZG+13, RCR+16, RO14b, RVP+11, SPL+18, SKKS13, STM+15, TLY+12, TNSS17, VVG13, Vor10, WdVN12, WNP+16, WZ17, WWW19, YZ16, YBS19, dRBO13, A1M+18, YZZ16, SHL+11]. ligand-based [RVP+11].

ligand-binding [GDV17, MGWR12, OSR16, RO14b, WWW19]. ligand-field [BBG+18b]. ligand-induced [KL14]. ligand-receptor [FRLN10, VKC10]. **ligand-sized** [OGL10].

ligands [CS17, GPdC+16, HRC13, KSO+19, LBC+19, LL10b, LXZ+10, LS11b, SSP+13, TS10b, ZRCC12, ZWY+10b]. ligated [EH13, WC14]. ligating [BAD+19]. **LigDockCSA** [SHL+11]. light

[FWS+18, GNI18, HXM+16, KDR+18, PE11, REL17, XBSS19, ZGZ19]. light-driven [HXM+16, REL17]. light-emitting [FWS+18, ZGZ19].

light-harvesting [KDR+18]. lighter [WD10]. Lightweight [RLG14]. like [AASP18, Che17, EPF+17, GRN19, KOY+12, KD18, KB14b, MP17b, OAN15b, SDF+17, SM15, UCFR16, VHA+10, VVY18, WFZ+18, WKC11, WGN+16, ZSL+11, VVY18, YLZ+19]. **Limit**

[SN16b, Fra15, Fra16, LW16, LYC+13, OAN15a, SLT14, WTH+16]. **Limitations** [LvG13a, VL19, HH18]. limiting [SLT+15]. limits [GC18, II18, NSK18, dLvNC18b]. **Linear**

[BG12, NNT+19, XKW18, YN15, ZLY+16, ARLP13, CPV+12, DSAS19, EP12, FBY+17, FCE15, GZZ12, JZZM14, JMS13, KHM19, Kid19, LF11b, MA17, MSAK12, NYH+17, PH17, RS17a, RLA+11, RR11, SS16a, Tak14, VBDS+11, WL10, YDX16, ZZZ+19]. linear-combination-based [Tak14]. Linear-scaling [BG12, YN15, NYH+17, RR11]. Linearity [IKN13].
lysine-malonylation [TYX+18]. lysozyme [ZP13].

[CAP17, CWZB10, Kne11b, LAT10, LAT11, PW12, RPNP10, RNP13, RR11, SS13a, STM17, TCPPC14, UIW+10, VVG+11, VKNT15, VKNT16, ZVY+15].

**matrix-based** [VVG+11]. **matrix-free** [ZVY+15]. **matter** [BGL+18, HRB+17]. **Maxima** [Lić14]. **Maximal** [DN19]. **maximum** [MLC13]. **may** [SMGB11]. **MB** [EdOdS18]. **MB-Isosteric** [EdOdS18]. **MBJLDA** [SRS14]. **MC** [HYUS11, BF19a, LH14a, ATIP18]. **MC-DFT** [LH14a]. **MC-QDPT2** [KKL+13]. **MCN** [LLL+11]. **MCQDPT** [LLSW14]. **MCSF** [ZZZ+19]. **MD**

[HCD+10, RSR+12, BM12, FB14b, GMASBF16, LWZ+19, LJL+11, MTvG12, OYK+11, RAR+11, SISK10, SMP17a, WTD+19, WWW19]. **MD-FEP** [LWZ+19]. **MDAnalysis** [MADWB11]. **MDLab** [CCW+10]. **MDM2** [HQS19]. **MDMX** [HQS19]. **MDockPeP** [XYZ18]. **MDTRA** [PVZ13]. **Me** [KKR+13]. **mean** [HDL+14, Kid19, KERY+16, KT10, KS12, KLS10, KMLS10, MIOM13, MP17b, RI10, VBDS+11, Vor12]. **mean-field** [Kid19].

**mean-force** [MIOM13]. **meaning** [PSP15]. **Means** [Sch18, KSM16, TBB+10, dSH19]. **measure** [TZCK18, WF16].

**measurement** [MPSG11]. **measures** [CDB10, CA10, Dry14, MK11, PZBA13]. **Mechanical**

[NN19, AC11a, APY+16, ACS12, ALH+10, BTT10, BEL+11, CXW14, DR11, DLW12, ECZW17, FL15, GMHH+16, HYUS11, Ibr11, JWO15, JSXH16, KVR10, LPE+10, MHRR11, NNK+16, NDD+10, OSR16, PML+12, PGW+17, PVAM16, Rez19, ŠBD+17, TZ11, VVV+18, VPR10, WKC+10b, WLL18, WCAH10, YKO+11, ZTI14, ZWMW10, ZKH+10]. **mechanical/effective** [DR11]. **mechanical/molecular** [BEL+11, YKO+11]. **mechanically** [SOY12]. **Mechanics**

[Ale19, AS10, AGB13, AS15b, BGR13, CGPP11, CXW14, Chu10, CHKR10, Cor17, CB11b, CB11c, DDM+15, EPH+13, ENKK+17, Fer13b, Fer13a, GEP+14, GPdC+16, HWLW11, KGHK12, LAHS16, LTP11, Lić14, Mat18, Min18, MS12, NLP+16, NKH+13, PSCI11, PGW+17, SFLG+17, VYM15, WOH16, WOH18, WCDM11, YPKB12, HWLW11].

**mechanics-based** [WCDM11]. **mechanics/dynamics** [DDM+15, EPH+13, GPdC+16].

**mechanics/generalized** [HWLW11]. **mechanics/molecular**

[ Fer13b, Fer13a]. **mechanics/Poisson** [HWLW11]. **Mechanism**

[GZL+12, SLY+10, SSC+19, VKNT15, WCWW11, WLF19, BHNS14, BMFG16, BEL+11, CPV+12, CPL11, CKG18, FWS+18, FB14b, GYX+10, GRCL12, GMSZ19, HYZZ13, HLI+19, HDH15a, HDH15b, HDH15c, JCG+10, JLS+10, JW16, KV14, KT12, KGJZ19, KS13b, KK19, LZL+10, LH111, LLB+12, LCC18, LWZ+19, LWXC16, LD18, LHT15, LPMT17, NJX+10, Oht16, PMLT16, RLG11, RSK+15, SLL13, SBW12, SZZ+18, VMTL10, WWW19, WQW10, WCL+11, XLY12, YPC+10, YHG+11, YYZZ17, ZWSL12, ZX19, vRET19]. **Mechanisms** [CGVBAI19, WJX+10, ZZWT12, DWZ+17, GG10, KC13a, MH11, MLY+13, PPH+14, RRFV+18, SLT14, SLT+15, SSP+19b, TNY18, Won18, WSWD19, YB11].

**Mechanistic**

[CYY+17, LZL+16, QQQ+18, TSJ+10, WFL+19, YZ17, YZLZ18, ABB+12,
[LLLW19]. MNX [AM19b]. MO [BRP+12, UIW+10, ZY14]. moana
der [DJD12]. mobilities [SFDE16]. Mode
[AIM+18, BHR15, GVP+10, IY18, SRA17, SBB10, YHCS11, YXZZ17].
Mode-tracking [BHR15]. Model [Ale19, BLS10, HM16, Jia19, MT20,
Pog10, AASP18, AOW11, AS10, ALRM18, ATP18, AS15b, APA+14, AB16b,
Bac12, BK17a, BH19, BEEL14, BS10b, BBG+18b, Cam15, Can10, Can11,
CGP12, CGA19, CBTZ16, CFC15, CAD16, CG12, CMS13, CJZS10, DLL+10,
DSF17, FCE15, FNSF+11, GRN19, GR515, GM17, Gil11, GKR13, HLS12,
HAL14, HLH+12, HOK17, HZSS17, Hug12, HRH+17, ISO+13, IN13, II18,
JSXH16, Jor17, KFY+13, KCK+17, KMS+19, KRY12, KOY+12, KD18,
KCPMG12, KB14b, KDS17, LSL+19, LTT16, LY10, LRvdSM15, LFN+10,
LPS+13, LHHW14, LZN+15a, LDG+15, LCK+18, LHMM11, MSLS10,
MT19a, MPJ+19, MBC11, MBC13, MB+17, MHO11, NXY+10, NTNY15,
OPBR17, PBY14, PCLL11, Pla11, Pon11, Ray13, RTS+13, Ric16, RMRRBH+19,
REL+14, RKG11, SM14b, SDF+17, SHF11, SSBW14, SK12]. model
[SK17, SLX+15, SDZ17, SZBM13, SB11, TYN15, TCC+13, Tia12, TLA10,
TKn19, UIW+10, VV15, VW+19, WWK11, WXL+12, WC13, WWW19,
WNM17, WHF10, WKC11, WCAH10, ZX11, XTY+14, XP13, YS18,
YMT14, YB13, YG12, ZST14, ZKH+10, ZM10, dSDdAR10, dSH19,
CCR18, FAS+18, MJBM12]. model-tuned [HZSS17]. modeled [MPA12].
modeler [BHI19, KLO+17]. Modeling
[ASW19, CB11a, DLSA14, FD13, FTW12, GMG+10, GBS+17, HPL13, JW16,
KDR+18, Mat14, NS10, NDLW13, PLP+16, SZdB19, SK11, Tia12, Vyb15,
AKMT11, Aou16, BEM14, BPC13, Bow16, BS10c, CMD13, CLA16, CZNA11,
DAG19, DWR17, DSX+11, DLLH12, EBPK17a, FXC+13, GH10, GP12,
GMZ12, GWJR18, GR10b, GWXZ12, HLvdV13, HBJ+17, JCL+17,
KSD+12, LABSG17, LLH14, LHZS11, LT13, MN15, MBB11, MLL14b, MA17,
MBA14, MPB11J, NSO+14, NW17, PHC13, PSS+17, PGM+16, QMK19,
RJS17, SN16a, SKGP19, TTR+12, VKN15, VAA14, VCM15, WXL17,
WPM+15, WLO+17, XDL+10, XLY12, YMY+19, YJ11, Zlx11, DHE+12].
modelling [DBM+15]. Models [Hes19, NNT+19, ND19, BEM14, BLKP12,
BPP11, CD11, Cor17, CBG16, CK17, DDP16, DSM+11, DI11, DGC14,
DL18b, EK15, EPD+10, GMP12, GBM+16, GMG+10, GKR13,
GCP+13, GCC14, GAJ+17, HS16b, HGY15, JC14, JGS+17, JKD12,
KCO+16, KBB1b, KR1+10, KSW16, LTT16, LKL10, LZ12, LSSW14, LM18b,
MPSA17, MSAK12, MUC15, MBK+13, NNS15, OLS13, PCH13, PGY15,
PL18, Ray13, RTP+13, RKG11, SPHF+18, SCMA+17, SFLG+17, SAVG15,
TH13, TTB+11, TLT+12, VKN15, VMS17, VZ14, WS10, WXY14,
WSW19, XTN18, YJ11, Y1L13, ZsA10, ZWD18, dSDdBNB17]. modern
[AB16a, AB16b, OH17, Fom11, LMR14, SF18, SDM+16]. modes
[CBP+15, EB18, GMP12, KKH18, LLTA12, MS17, dSH19, dSAdSL13].
modification [Ano12u, MI+15]. modified
[BD12, CH16, DPL16, DJ+11b, GSD10, MRO17, Mit13, SMM15a,
SMM15b, SM+18, XYX17, XVA+16, ZZ12]. modify [ZX19]. Modifying
modular

Modulating

molecular

molecular
nanostructure [LLD17]. nanostructures [ZZY17]. nanosystems [PGK19, Tia12]. nanotube [AJA19, ASI5a, FTR15, JWO15, KHE19, OCW15, RHNN10].
KWL+16, KK17b, KWG15, KYG+15, KAG+12, KSW16, KPF+15, LPS12, LJR+12, LHS12, Leh15, Lr1dSM15, LrV17, LDB+17, LLAZ12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MDT16, MBR+15, MYT18, MSSH17, MB14, MB16, NKJ16, OV14, OPB+12, OZS+13, OC14]. News

[PPS14, PGL+15, PSN+17, P12, PPM15, PHH+12, PVZ13, PG14, RLLH12, RNSF+16, Ras17, Rez16, RR14, RDS12, RCM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sic15, SJ17, SWB+12, SDMS13, TNYN16, TSC+13, TTR+12, TTL+12, UU12, VRMRS+17, VVV+15b, VAR12, VBV13b, WV12, WDV13, WPD+15, WF16, Wei12b, WHK+12, WHJH13, WG14, WCP+14, XML+15, XY+17, YWJ+16, YZZ16, Yes12, Yes15, YHH+13, ZDK12, ZLL+13, dVAG16, KKR+13]. Next

[ADF+10, HGY15]. next-generation [HGY15]. NF

[ABB+13, ABB+12]. NGuaS [WGN+16, WGLG+16, WRG+17]. Nguyen [Ano15-59]. NH


[Ben17, CHP11, EOA+11, HJ13, HBI+17, HM13, KASH14, LKI11, OPR16, PTK11, PGoD+16, PCl14, Pie14, RK15, SPH+18, SEF+16, SKMS13, SPZP18b, SPZP19, Ts19, TED18, WL14, YS13]. NNO [WGL+11]. NO

[MCU15, Ts17, ZZI0, WYW12, BS16a, GY12, LWZ+19, MN19, OSH17, RGV+19, TNI+19a]. Noble

[BGS+19, SM18, ARLP13, GC18, JKS+16, PG5+15, PMG+16]. Noble-Gas [BGS+19]. NOCV [CSM16, DBGO+17]. node [KK17a]. nodes [FSSW19, KPF+15, KPF+19]. NOEs [LK11]. Non

non-equilibrium [NHN16]. non-heme [PHC13]. non-hybrid [CSKH15].
non-natural [GMZ12]. non-uniform [YWJ+16]. nonadditive [RTS+13].
Nonadiabatic
[HZ11, RGVC+19, JBSQG11, KIOY19, MT19b, SRSLO15, WLF19].
nonadiabaticity [Wu10]. Nonbonded [ND19, Abr11, EP10]. Noncatalytic
[SGS+16]. Nonclassical [GZ11, RGVC+19, JBSQG11, KIOY19, MT19b, SRSLO15, WLF19].
nonadditive [RTS+13]. Nonadiabatic
[HZ11, RGVC+19, JBSQG11, KIOY19, MT19b, SRSLO15, WLF19].
nonadiabaticity [Wu10]. Nonmetal
[ZLX+19]. nonorthogonal [ZM11]. nonparametric [RB13a].
nonperiodic [MS15]. nonplanar [KG11]. nonpolar
[LvG13b, MPAA17, PAT+10, WWWW18]. nonpolarizable
[AOW11, WG12, ZRL+15]. Nonrandom [NPP13]. nonredundant
[HZ13, MK19]. nonresonant [BZB+13]. nonspecific [CBP+15].
Nonstatistical [Yu12a]. nontemplate [OL13]. Nontotally [HOM+16].
nonuniform [BD12]. norbornadiene [Ant13, WJX+10]. Normal
[BY18, GVP+10, GMB12, KKH18, MS17, SBB10]. Notes [CD13]. Novel
[FCL+10, KKO+16, RPNP10, AIGP15, BEPM14, BPM15, DWW11, DMN14, DFF+15, JYS+12, LLLC11, LLLJ12, MPNS13, PSED1+10, RNP13, WFS19, WKC11, YJN+11, YHCS11, YDGY15, dCLFGL13]. Novic [CD19]. novo
[AFBR17, BAMR13, LK11, MDT10]. Nuclear
[ASK18, DKT13, ECZWD17, KNP+12, CSEMB+16, HH16a, HH17, JKS+16, MT19b, NASH15, PLFS18, RSG14, SPHF+18, SS13b]. Nuclear-relaxed
[ECZWD17]. nuclearity [BACSCJ+10]. Nucleic
[HGY15, ZWP11, Fel10, FCE15, GRE11, MSLS10, OXWB16, SCF+19, SGG+18, SWB12, WGT12, XNY17, ZSB+11]. nucleic-acid [SGY+18].
nucleobase [ANH+11]. nucleobases [CC18b, WG12, ZB18]. nucleophile
[ZYR+15]. Nucleophiles [WBKS19]. nucleophilic
[JDS+19, MA16, MLY+13]. nucleophilicity [TMJ15]. nucleotide
[CBG17, MJDC14, Ran13]. nucleotides [DMN14]. Nucleus
[ZBB16, FBB10, TH13]. Nucleus-independent [ZBB16, FBB10]. nudged
[QB10, QB11, SH11a]. null [TTn19]. null-space [TTn19]. Number
[Ant10b, ASMS10, CLK11, DSV+19, GPM17, HMM10, MEH18, SL10, SG10b]. numeric [VI17]. Numerical
[WXL17, CKKK16, KEMP17, KP11, MABA11, SSK19, SLG15, YSG12].
numerically [ZDM13]. NUPACK [ZSB+11]. NWChem [PGW+17].
nylon [BHNS14]. nylon-oligomer [BHNS14].
O [AM19a, BCN+11, CXS10, CSNCS+18, DHE+12, GBGR16, HRL11,

packages [MSvG12, MJG15]. packet [LWD13]. packing [MCAG16, MP17b, NS11].

**PaDEL** [HLS13, Yap11]. **PaDEL-DDPredictor** [HLS13].
**PaDEL-descriptor** [Yap11].
**PAEM** [ZY14]. **PAEM-MO** [ZY14].

**pair** [BSF18, BH13, CYG15, CVG14, Hei18, KS18, MPA12, OM12, Sch12, SSIG15, SB14, TNY18, WCY11, WWU12]. **Paired** [ZR10, WAB17].

**pairing** [KTK17, ZLL10, ZM11].
**pairs** [BSG18a, DKT13, ENKK17, LEdOLdlV17, LZH11, MPSG11, Mau14, PL19, GMBM18].

**Pairwise** [GS14, Gon12, RVMPS17, XTY14]. **pairwise-additive** [VMPS17].

**palladium** [MRC18, WCWW11, YHG11, dCDP15]. **palladium-catalyzed** [dCDP15]. **palladium-phenanthroline** [MRC18].

**paper** [GPGSM12, Ihl12, JW12, WM12, HP10a]. **para** [KYCL11].
**para-substituted** [KYCL11]. **paracyclophane** [KGR16]. **paracyclophane-bridged** [KGR16]. **Paradoxical** [UT14].

**Parallel** [BTB11, FBKD19, KDB13, NN18, UIW10, WWKS16, BW11a, BTT10, CEB015, CSSB11, GJMPAM14, GRARO14, GC18, HP10a, HS17b, HPSK12, KS13a, KNH16, KN17, KZZ16, KCC18, KJM17, KDT12, LI10a, LPLA13, MR15, MCRL17, MYT14, MJM15, NNK16, OPB12, RFN15, SHM011, TCTX13, TJB12, WHK12, Yes15, ZWL13, ZSS13, CCL13, KDT12, LMR14]. **parallel-generalized** [LL10a].

**Parallel-ProBiS** [KDT12]. **parallelism** [FRN15, Gon12]. **Parallelization** [AB16b, RC18, VDL13, BWMSM10, IUK11, JMS14, KS15, KKK11, LLZA12, RSRR15, SLH19, vW11, ZDKM12]. **parallelize** [vW11].

**Parallelized** [AIQ19, DBDP16]. **parallelizing** [BMBJ11]. **parameter** [NB19, PFVL14, SH19a, VCL18, VVLG17, WDZH13, LL11].

**Parameterization** [HK18, HJJLV16, ILKR11, IHJ13, MPSA17, PRRT10, TCC13, BAS14, CCLP12, DLH12, KYB13, LTP11, LCL18, MSS13, VLB10, VBD11, VHS19]. **parameterizations** [SH15]. **parameterized** [OZS13]. **Parameters** [CTR13, AG11, AKMYB18, BCSCJ13, BCJC14, BSD18, BW15, BC13, CYG15, DPSL16, DMAH15, FHT15, GSD10, HLS12, HM16, HBI17, HLH12, KvdV14, GKH12, KJZ19, LVDH13, LPS13, LLvG10, LSH11, MRO17, MP11, PBL19, Pog10, RKB14, SOYC12, SBB13, SPR13, SPZP18b, VYM15, VLGK17, WAM17, WOH16, WOH18, WC14, YZW14, ZRL15]. **Parametric** [LM18b].

**Parametrization** [PG15, COHI19, DGPM14, GCWS15, SPS12]. **Paramfit** [BW15]. **parasite** [FZL15]. **paratropic** [CPN17]. **Parrinello** [DL19, KCK15]. **Part** [HRJ15, CDBM11, CD13, HRJ14, Fer13b, SK13].

**Partial** [HTS17, JMLL13, SMP17b, WOH16, GVG10, MPBJ11, PL14].
**Partially** [Xtn18, UT14]. **participating** [GSMZ19]. **particle** [AG11, BSD18, BK13, Cas13, ER18, Hei18, NO16, PH17, RJBH18, SCK18, ZDKM12]. **particle-field** [ZDKM12]. **particle-mesh** [AG11]. **Partition**
[LRVM18, HGCCGR+16, JIS13, LRER13, WG12, WDHZ13, WZWW18, YAS13]. **Partitioning** [VSP19, DK11, EV14, FCOGM12, FHZA+18, LZS+17, REL17, SS13a, TMJ15, VGV+11, ZW18, VV19]. **partner** [dVZ17]. **pass** [SR18]. **passing** [CSSB11, ZWL13]. **Past** [GS16, MFEM16, XFG+16]. **patches** [OME16, YSSB12]. **Path** [MA17, VKAM12, CY09, DL19, HXM+16, Ish10, JZ17, KSNT19, MvBD18, SRSLO15, SA13, SS13b, SMM17, TN18, TNY18, WXY14, ZT14, MYKO18, CY13]. **path-based** [ZT14]. **Path-integral** [VKAM12, WXY14]. **path-search** [Ish10]. **PathOpt** [GPE13]. **Paths** [SH11a, AMGB10, Ant13, CX10, Jab18a, NMLD13, RVP+11]. **pathway** [BHB12, HOM+16, LKL10, SJD14, TDP+12, XLYZ10]. **Pathways** [JL19, CM13a, EF5B16, GS11, HNTS15, KGR+16, KDR+18, MTM14, NJR18, QSW+10, QB16, RCM+13a, RML+15, SJD11, SH18b, Tisi17, WSH10, Yon16, BHB12]. **pattern** [CXS10, LZSM19, WGL12]. **Patterned** [SJSS19]. **Patterns** [KKGW19, FZL+15, RS14]. **Paul** [Ano15-60, Ano16-56]. **Pauli** [JJH+13]. **PAW** [LGKS17, MDTD13]. **PAW-based** [LGKS17]. **Pb** [MCK17b, PMG+16, vSGP10, FBY+17, OBW12, VM11, vSGP10]. **PB-AM** [FBY+17]. **PBE** [DOM+11, PTK11, LKL16a, SGPSJ+17, TG12a]. **PBE-QIDH** [SGPSJ+17]. **PBE/3z** [PTK11]. **PBE0** [DOM+11, LKL16a, SGPSJ+17]. **PBE0-DH** [SGPSJ+17]. **PBESOL** [DOM+11]. **PbI** [VVY17, VVMY18]. **PbS** [NS18]. **PBSA** [BD11, CS17, RDDS10, STM+15]. **PBSS** [DVVP14]. **PC** [VL17b]. **PCASSO** [LFB14]. **PCCP** [VT14]. **pCCSD** [Sch12]. **PCM** [LFN+10]. **PCM-MST** [GMMH+16]. **PD** [HLS+13, Hill13, KD10, Niz13, YDR13, dSdLBNI17, GA19]. **PD-PK-T** [HLS+13]. **Pd** [GA19]. **PDB2PQR** [UHH+11]. **PDBbind** [PLAG11]. **PDECO** [CJL+13]. **PDielec** [KB16]. **PDixCN** [ZZL19]. **peaks** [LZS+17]. **PEG** [EOO+16]. **PEG-PLA** [EOO+16]. **penalty** [GZH10, LL19b]. **penetration** [NLP+16]. **penta** [dCGCRN19, LBC+19, Sak18]. **penta-coordinated** [Sak18]. **penta-coordination** [LBC+19]. **Pentaatomic** [XhD15]. **Pentacene** [NNT+19, CWHH11, ZYG+15]. **pentacoordinated** [TS10b]. **pentagon** [FL15, GZH10]. **pentane** [TCGNT18]. **pentaprimane** [PCLL11]. **pentathienoacene** [ZYG+15]. **penten** [LXF17]. **peptide** [FP17a, HHNK19, HPL13, HLY+12, IC$^+$12, IC$^+$13, JBAM11, JWST10, LTT16, LW11, LlVgo10, LjW+11b, LVg13a, LMA15, MDT10, MV17, OZ14, QZM11, SV15, SEM12, SZB19, TYZ+16, WS19, XHL16, XYZ18, YZ15a, dLFG113]. **peptide-backbone** [HLH+12]. **peptide-design** [XHL16]. **peptides** [BLKP12, BPC13, CR19, COOH14, CZNA11, GFG11, HSB+19, HLH+12, HWWL17, IO13b, JX10, KB10, LvG13c, MZZ11, MUGNVJ+18, OLY17, WNM17, XHL16, XWSW13, ZKH+10]. **peptoid** [MMZW14]. **peptoids** [WS19]. **perception** [AJR16, HYYZ13]. **Performance** [Abr11, BZB+13, CSHK16, CKKK16, DAP+18, DOM+11, GWRJ18, HSB+11, HB19, JCP14, LK16a, RKB+14, SF18, SH18a, SGWA17, ZZMW19, ABM+15, BLBG+13, CLF018, CXS10, CSSB11, CJZS10, ES13,
SHL^{+18}, SLX^{+15}, ŠSB^{+16}, SJC11, SGHL13, VCL18, YB16, ZL11.

powdered [KB16]. Power [Min18, LZL^{+15a}]. powerful
[CAT^{+13}, HMO^{+18}]. powers [WZ17]. pp [CD19, Spr10]. PPI
[RMRBH^{+19}]. PPI-Detect [RMRBH^{+19}]. PR [TTB^{+10}]. Practical
[GR10b, SLG15, BB11b]. pre [RLDJ17]. pre-computed [RLDJ17].
preadSORbed [KD10]. prebiotic [SSNT19]. precatalyst [MJLV14a].
precatalysts [MJLV14a, MJLV14b]. precision [DH17, MLC13, SWW^{+19}].
predict [ASMS10, CBH14, DLC18b, HWB19, LLSW14, SEF^{+16},
SPZP18a, WJG^{+13}]. predictability [BBOB16]. predictable [GDV17].
predicted [DWL11, LZW^{+11}, TYX^{+18}, WKLC12, YZ16, Zha12b, ZWX19].
Predicting [AS14, AS18, BVHI17, BB11, cCVG^{+14}, CPK19, ELKE19, GC18, GRL^{+11},
JGS^{+17}, Jor17, LZSM19, LDH^{+14}, PgDo^{+16}, RDF^{+11}, SJWE10, TYX^{+18},
VL19, YZ15a, DBM^{+17}, Kar17, KTO13, RB13b, SMDP18, SIG^{+11},
WCDM11, Yon16, Zha12b, Zha12a, ZLX^{+13}, ZYS^{+10}, GRL^{+12}]. Prediction
[Ano12u, AIM^{+18}, CP15, CQFC10, FSD^{+18}, HZSS17, KPL15, LDZW17,
MCAG^{+16}, vOaCG10, PRP15, SRA17, SPL^{+18}, WDW12, YHW17, ZYL^{+12},
AGM^{+13}, BLDK^{+13}, Ben17, BddS13, BA11, CZAFL7, DLW11, DDP16,
EOA^{+11}, FZY^{+12}, GK10, GFPSD17, GTZ^{+18}, HLS^{+13}, HPL^{+18}, HYMZ16,
HL14, JSW10, KL14, KT10, KTO11, KB19, LXL^{+11}, LMI^{+14}, LZL^{+15a},
LZZ14, LLH11, Lwl^{+10}, LSH^{+11}, MDT10, Mau14, MG11, MSÃ K12,
PML^{+12}, PN13, PJP14, PLV^{+11}, RCR^{+16}, RMRBH^{+19}, RBK^{+14}, SM11,
SYH12, SSD19, TYZ^{+16}, VKC10, WLF11, WH11, WXS^{+12}, WXL^{+12},
WWW18, XFTW15, YVEI^{+17}, YLCX10, YHH^{+13}, YDX16, YDgZ15,
ZsA10, wZbZ11, ZYvIZ14, ZLW10, ZHHX11, ZDW18, MSP18, SIG^{+11},
WCDM11, Yon16, Zha12b, Zha12a, ZLX^{+13}, ZYS^{+10}, GRL^{+12}].

predissociation [YB11]. Preface [GS18]. preference
[DSHLM18, LKZM18]. preferences [FCOGM12, LGL11]. preferential
[TKYN17]. preorganized [CM16]. preorganized-interacting [CM16].
preparation [JSD^{+11}]. present [Cas14]. presenting [ZGZ19]. preserving
[WBKS19, CCJC10, DBM^{+15}, LLB^{+12}, MCF10, SBGP18, Tak11, YPvD13].

Predictions
[Ano12u, AIM^{+18}, CP15, CQFC10, FSD^{+18}, HZSS17, KPL15, LDZW17,
MCAG^{+16}, vOaCG10, PRP15, SRA17, SPL^{+18}, WDW12, YHW17, ZYL^{+12},
AGM^{+13}, BLDK^{+13}, Ben17, BddS13, BA11, CZAFL7, DLW11, DDP16,
EOA^{+11}, FZY^{+12}, GK10, GFPSD17, GTZ^{+18}, HLS^{+13}, HPL^{+18}, HYMZ16,
HL14, JSW10, KL14, KT10, KTO11, KB19, LXL^{+11}, LMI^{+14}, LZL^{+15a},
LZZ14, LLH11, Lwl^{+10}, LSH^{+11}, MDT10, Mau14, MG11, MSÃ K12,
PML^{+12}, PN13, PJP14, PLV^{+11}, RCR^{+16}, RMRBH^{+19}, RBK^{+14}, SM11,
SYH12, SSD19, TYZ^{+16}, VKC10, WLF11, WH11, WXS^{+12}, WXL^{+12},
WWW18, XFTW15, YVEI^{+17}, YLCX10, YHH^{+13}, YDX16, YDgZ15,
ZsA10, wZbZ11, ZYvIZ14, ZLW10, ZHHX11, ZDW18, MSP18, SIG^{+11},
WCDM11, Yon16, Zha12b, Zha12a, ZLX^{+13}, ZYS^{+10}, GRL^{+12}].

predictions [ALK^{+15}, BCP^{+10}, CLA16, CS17, EOO^{+16}, GAI13,
KZK^{+12}, PdSc18, RDDS10, RCM^{+13b}, SHMO11, SA10, WZW18].
predictive [LLL^{+10}, WKC11]. predictor [CDS16]. predictors [GHK12].
predissociation [YB11]. Preface [GS18]. preference
[DSHLM18, LKZM18]. preferences [FCOGM12, LGL11]. preferential
[TKYN17]. preorganized [CM16]. preorganized-interacting [CM16].
preparation [JSD^{+11}]. present [Cas14]. presenting [ZGZ19]. preserving
[WBKS19, CCJC10, DBM^{+15}, LLB^{+12}, MCF10, SBGP18, Tak11, YPvD13].

Pressures
[YAO18, AYYO17, Cam15, CCR18, FCW^{+14}, HYNS19, HHRI17, II18,
LLL^{+12}, MO17, NFPD13, SMDP18, SPZP18a, WDLG12, CCR18].

pressures [RHNN10]. primary [ALK^{+15}, GAI13, VVLG17, KTN110].
prime [DSX^{+11}]. prime/MM [DSX^{+11}]. primitive [HAL14]. principal
[PSP15]. Principle
[WBKS19, CCJC10, DBM^{+15}, LLB^{+12}, MCF10, SBGP18, Tak11, YPvD13].

Principles
[HFSO12, BE12, BE14, BPE16, EMD17, EB12, EBK13, EBPK17a, EB18,
GD10, HYL^{+11}, Ibr17, JCG^{+11}, KLZ^{+18}, LLLM11, LCWW10, NNS15,
OC19, PLZ17, RZG^{+13}, SFA17, SPZP18a, TZ11, UGK18, WYL^{+15}, WD10,
YR13, wZbZ11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC^{+14}, THI^{+19}].
proteins [SCF19, SB11, SIT18, SLIB12, SWMW10, SZB19, SZZ18, SIG15, SGH16, TN12, TFQ10, TFQ11, TS11, TS15b, VPR10, VECT12, WLC12, YW12, YCGA10, wZbZ11, ZYG15, ZWMW10, ZB18, ZLX13, ZBP11, ZYL12, ZGZ19, FDCJG18, SFCCK15].

property [CD13, GPS10, GBS17, GWX12, PH15, V˚AA14, WH11].

propionate [TN10].

propionic [CM16].

Proposal [PRYI17].

proposed [GS11].

protease [DLZ15, NHN16, OBW12, SYH12].

protective [JAH17].

Protegrin [RI10].

Protegrin-1 [RI10].

Protein [CIKT13, CDS16, CPK19, DPOS16, GPS10, HNTS15, HS16b, JL19, LZGS11, MFEM15, MFR10, PGL15, Ran12, RP15, Rao11, SHMO11, SKKS13, YBS19, AIGP15, AKK16, AM10, AG12, BSZ12, BFH13, BBP11, BPC13, BCG10, Bow16, BDiS13, BA11, CSC18, CZAF17, CFC15, CHR12b, CHR12a, CM13b, CCYL11, CKP10, CH14, CC12b, CBG16, CHP11, DWL11, DJ13, DVP14, DLMI12, ESD18, FZY12, FHW11, FCE15, FLM11, FSC14, GS14, GDV17, GMS1G15, GRP12, GZ14, GRL11, GRL12, HAGK10, HNHR13, HMO18, HTS15, HTS17, Has14, HZY10, HPL18, HKR12, HYMZ16, HJ10, HBY10, HM13, HZ13, HZ14, ILKR11, HHY15, JZ12, JZZM14, JL17, KTY17, Kan15, KNE11a, KOY12, KL14, KERY16, KJ10, KTO11, KTO13, KDT12, KLS10, KMLS10, LS11a, LFB14, LHL10, LH11, LCPS13, LC16, LC17b, LZ11, LL10, LL10b, LFM12, LPS13].

protein [LZZ14, LLLC11, LHG11, LBS10, LM18b, LL19b, LDH14, MS17, MMM16, MJ14, Mau14, MUGNV18, MA17, MFEM15, MS16, MP11, MKB13, MOS12, MNNK10a, NSK18, NST14, NS11, NFG13, NG10, OHNK11, OCL11, CPL10, CH14, CC12b, CBG16, CHP11, DWL11, DJ13, DVP14, DLMI12, ESD18, FZY12, FHW11, FCE15, FLM11, FSC14, GS14, GDV17, GMS1G15, GRP12, GZ14, GRL11, GRL12, HAGK10, HNHR13, HMO18, HTS15, HTS17, Has14, HZY10, HPL18, HKR12, HYMZ16, HJ10, HBY10, HM13, HZ13, HZ14, ILKR11, HHY15, JZ12, JZZM14, JL17, KTY17, Kan15, KNE11a, KOY12, KL14, KERY16, KJ10, KTO11, KTO13, KDT12, KLS10, KMLS10, LS11a, LFB14, LHL10, LH11, LCPS13, LC16, LC17b, LZ11, LL10, LL10b, LFM12, LPS13].

protein-bound [FLM11].

protein-coding [YS10].

protein-coupled [ILKR11].

protein-glycosaminoglycan [SZdB19].

protein-ligand [AG12, CHR12b, CHR12a, LLC10, OOT15, SPL18, WdVN12, dRBO13, AIM18].

protein-like [KOY12].

protein-lipid [PGCT12].

protein-peptide [XYZ18].

Protein-protein

[GS10, HOSZ19, NG10, PBL19, RMRBH19, WLLL18, WES13, WHAS10, WHAS16, XML15, XYZ18, YZ15a, YZ16, YDL10, Yon16, YS10, YL13, ZC14, ZYV14, ZLW10, ZLX13, ZDT18, ZSB16, dRBO13, AIM18, DKV18, LGL11, SL10, SHL11].

protein-RNA [HZ13].

Protein-specific [CIKT13, JZZM14].

proteins [ABD11, CTR13, CGBK13, DMJ17, FZL15, FP17b, FBEM11, HS16a, Ham11, HTS15, HTS17, HS17b, HYN19, HRC13, HS14b, HRH17, JC16,
python [SH19b, HPT+16b, LRvE17, PHH+12, SHFJ18, TBJ18, Yes15].
Pytim [SHFJ18]. PYX [LWWG12].

Q [WPM+15, BS10c, GKV+13]. Q-CHEM [GKV+13]. Q-Dock [BS10c].
Q2MM [LN15]. Q5 [REL+14]. Q5/D5Cost [REL+14]. QB3 [KG15].
QikProp [LP11a]. QM [BM12, Lun12, RSR+12, Lun12, PLP+16, AALCM11, BH13, BZH14, CBG17, CJZS10, DSK17, FRC18, FLM11, FB14b, GR15, GZ15, GCW14, HH15, HYUS11, HBR17, JJH+13, JWST10, Kid19, KTN10, KWL+16, KG15, Lzdl+10, LFM12, LT13, LHT15, LJJ+11, MCR17, MTvG12, MJG+15, NO16, Q5 [REL+14]. Q5/D5Cost [REL+14]. QBB3 [KG15]. QCSA10, TSC+13, UT11, VKNT15, VKNT16, VCM15, VKTR15, WDP+12, vRET19, GRS15, JAH17+19, LWZ+19, RFN15, ZZY+16].
QM-only [LT13]. QM/QM [GRS15, JAH17+19, LWZ+19, RFN15]. QM/EFP [CBG17]. QM/MM [BM12, RSR+12, AALCM11, CJZS10, DSK17, FLM11, FB14b, GZ15, GCW14, HH15, HBR17, JJH+13, JWST10, Kid19, KTN10, KWL+16, KG15, LFM12, LT13, LHT15, LJJ+11, MCR17, MTvG12, MJG+15, NO16, OYK+11, PMC+17, P10, PDMT10, PL14, PLP+16, RR14, RGR12, SN16a, SGDT10, SJ14, SCM+15, ST15+1, SASS10, TSC+13, UT11, VKNT15, VKNT16, VCM15, VKTR15, WDP+12, vRET19]. QM/MM-QMC [UT11]. QM/MM-type [Kid19].
QSARINS [GCP+13, GCC14]. QSARINS-chem [GCC14].
QSAR/QSPR [CD13, BRN12, CLX+10, CD13, CD16, GCC14, KKO+16, TTR+12, XWW+11, YMY+19]. QTAIM [BH13, BZH14, FC112, FCP114, GMX+16, HXX+16, JX1+16, dR11, Rod13, RSKG14, VV15, Wei12b, WvRSM14, XFX+16, ZZZ+12, ZCW18, dLC18a]. QTAIM- [VV15].
QTAIM-based [FC112, FCP114, Wei12b]. quadrupolar [CSE16]. quadrupole [HB10, LL16]. quadrupoles [NL16].
Quantitative [YK13]. Quality [CLK11, KCK+17, KYY13, LOB18, MCF+18, MK+13, OLB19, POB13, RB13a, RC13b, SC15]. QuantPol [TSC+13]. quantification [Fer17, Ham11, PC14, SKGP19, YNH+17]. quantify [LLH16]. Quantifying [TMJ15, GMX+16, MS10]. Quantitative [DZA11, RTD14, VAA14, Wei12b, BCP13, CD13, DXL+10, NFG+18, NFG+13, REL17, RC13b, XFW15, TTT+11]. Quantized [KK19].
Quantum [ALK+15, AC11a, APA+14, CH10, CG12, DDM+15, FRN15, GH10, HHD+16, JCT18, KASH14, LL14a, LL14b, LW13, MM18, Mat18, MB16, MS12, NNT+19, NN19, OKY18, RFN15, SCOJ13, SAGC16, SBD+17, SOYC12, SR10, SHB17, TR12, UD12, VP19, VSP19, WCA10, 100]
WDP+12, YHX19, Aki16, ATP18, ASS+17, ARAG17, AAC+16, APY+16, ACS12, ASK18, ALH+10, Bac12, BTT10, BRP+12, BGR13, BEL+11, Cam15, CBH14, CD10, CDB10, CDBM11, CD13, CD16, CDC19, CXW14, CHKR10, CSNCS+18, CM16, CKG18, DR11, DKT13, DDP+18, DPAB16, Dra19, ECZWD17, EV14, Fer13b, Fer13a, FB10, FFA14, FC18, FLN11, GPM17, GM16H+16, GTK10, GGM+12, HZ11, HSN+18, HLvdV13, HPT+16b, HGCCGR+16, HMM10, HYUS11, HGY15, JBB+11, JSXH16, KP11, KNR+18, KVR10, KKH18, LPE+10, Luc14, Man19b, quantum [MP17a, MAPB10, MSvG12, ME10, MSSP17, MHRR11, MFR+11, NC13, NC14, NK+16, NDD+10, NHK+13, NS17, OKIS17, OR16, PML+12, PNE18, PSC11, PGW+17, PBG17, PVAM16, RLLHL12, Rez19, REL+14, SLT14, SKA19, SS13b, SPZP19, Tac19, Tsi18, UK+18, VPR10, VBA13, WKC+10b, WBT10, WLLH18, WAB17, XCLZ19, YKO+11, YLS19, YW13, YKH15, ZW17, ZVY+15, dCDP15, BLG10, OSI+19, SKA19].

Quantum-chemical [KASH14, FB10, MSvG12, MFR+11].
Quantum-chemistry [DDM+15].
Quantum-classical [HLvdV13, SKA19].
Quantum-mechanical [ACS12, ECZWD17, PGW+17, Rez19].
Quasi [YLT+19].
Quasi-planar [YLT+19].
Quasiclassical [YLT+19].
Quaternary [DSHLM18].
QuBiLS [GJMPAM+14].
Quest [AOW11, EK17].
Questions [BZH14].
Quick [VVV+15b].
Quickly [vW11].
Quinacridone [HSZ+11].
Quinoline [HRJ+14, HGHP14, HRJ+15, JRSHP14, SSD19].
Quinolone [ZCK+16].
Quinone [GLM+17, VSD10].
Quinones [uLhY11, SDIP18].

R [LdSRR16, LTR18, NDG14, Sch10, DJS+18, GA19, LdSRR16, LTR18].
R-C [LdSRR16, LTR18].
R-Group [LdSRR16, LTR18].
R-NHC [GA19].
Radial [ME10, COHI19].
Radial-template [ME10].
Radiation [LZH+11].
Radiation-damaged [LZH+11].
Radical [AAMD+11, GAI14, GKR13, JCG+10, KGR+16, KV14, LJG+11, MUN+19, PNE18, Ray13, RKG11, SDJ11, TTR+12, TL16, WHLI11, ZZL+10b, ZL14, ZSZ+14, dLC17, CPR18].
Radical-bridged [ZLZ14].
Radical-formic [TL16].
Radical-molecule [GAI14].
Radicals [CGVBAI19, Den12, KS13b, LG19, SRR16, WCT+11, WHLZ12, ZZL+10a].
Radii [STM+15, YOMT14].
Radio [AB10].
Ragüé [Ano16-56].
Ramachandran [KS12, MP17a].
Raman [EB18, PAK15, SLLL13, YB13].
Randić [CD19].
Random [HMM10, AC11b, CY09, CY13, CLK11, GPM17, OLA15, RDRC16, WZ17].
Randomized [JCPIC11].
Range [CKH19, Ali18, AO10, BLBG+13, BCNH+11, BK17b, CSK15, ELF19, HH15, HZZS17, Jan16, KKH19, KB10, KSH13, KSSH13, MMS16, NLP+16, RSG14, Rui11, SGMB11, SH18a, ST13, SPH11, SH19a, SZB19, ZZS16, SSA+17, VL17a, VCL18, WY17].
Range-separated [Ali18, BK17b, HZZS17, RSG14, SH18a, ZZS16, WY17].
Range-separation [VCL18].
Ranges [MA12].
Rank [EPD+11].
Ranking
[KERY$^{+}$16, HWLW11, MP11, PBG17]. Rapid
[LJW11a, LW11, LAT11, MZZ11, MRR11, MSS$^{+}$13, MFR$^{+}$17, NO16, PG14, 
RZ16, TM18, JSW10, KLOS10, DK11, WBF17]. Rapidly [OPR16, RDRC16].
RAQET [HSN$^{+}$18]. rare [HNS16, LRvE17, MP13, Sea10, STS15]. rare-gas
[MP13, Sea10]. RASPT2 [BH19]. Rate
[AR10, AAMD$^{+}$11, CSNCS$^{+}$18, NMLD13, CBH14, GAI13, GKR13, HSL$^{+}$11, 
JWO15, KB19, KCL$^{+}$14, MSV16, MK17, MK19, NDW15, OZLSBH12, 
RAGLL11, Ray13, RKG11, SSC$^{+}$19, STM17, TTR$^{+}$12, ZLL$^{+}$10b]. rates [BL12, CSAdOM17, GRL$^{+}$11, GRL$^{+}$12, QB16, SHB17, WAB17]. ratio
[BB11b, KB11c, ST13, dRBO13]. Rational
[CSC$^{+}$18, NPG$^{+}$18, Spr18, SCSM19]. rationale [AARP17]. Rationalization
[TLdG$^{+}$12, SLC$^{+}$17]. ratios [OZLSBH12]. Raton
[CD19]. rats [TTB$^{+}$11]. Ray
[CPR18, FLM11, LLBO12, LSHH12, MKK$^{+}$19, PDG$^{+}$16, WWD14, XML$^{+}$15].
Rayne [GKR13]. Rb [YLT$^{+}$19, ZWY$^{+}$10a]. RbLi [DHOG13]. RC [YKH15].
RDG [VVJ15]. RDG-based [VVJ15]. Re [FD16, KSC16, DLW12]. Re-evaluation
[KSC16]. reach [QZ10b]. Reaching [MCRL17]. Reaction
[DBGO$^{+}$17, FB14b, HSL$^{+}$11, IT19, LWL$^{+}$16, LWZ$^{+}$19, NIX$^{+}$10, QSW$^{+}$10, 
QB16, ST13, AMGB10, AS11, Alg17, AR10, APA$^{+}$14, BK15, CYY$^{+}$17, 
CSAdOM17, CXW14, CSNCS$^{+}$18, FB12, GYX$^{+}$10, GZL$^{+}$12, GTK10, 
GKR13, GJ17, HOM$^{+}$16, HL13, HJL16, ITY$^{+}$19, IIF$^{+}$10, JZ17, JLS$^{+}$10, 
JW16, KV12, KV13, KL15, KSK11, KK19, LGOM$^{+}$15, LZY$^{+}$12a, 
LJW$^{+}$11b, LZL$^{+}$16, LW131, LPM17, MT214, MHT$^{+}$18, MPSG11, MS10, 
MJLV14a, MJLV14b, MTS$^{+}$19, MT19b, MB16, MMJ10, NH19, NMLD13, 
NMI19, NTTY15, OA19, OZLSBH12, PVL$^{+}$13, PG18, PNE18, PPH$^{+}$14, 
QYL10, RAGLL11, Ray13, RLZ$^{+}$18, RLS13, RRFV$^{+}$18, RN17, RKG11, 
RSG14, RSK$^{+}$15, SLT14, SLT$^{+}$15, SJD14, SRF$^{+}$17, SBD$^{+}$17, STS$^{+}$10, 
SSP$^{+}$19b, SMM17, SM17, Tac17, Ta14, TN18, TNY18, TSJ$^{+}$10, TDP$^{+}$12, 
TCPPC14, Tsi17, VBD11, VV14, VGT16, VMT10, Wu10, WHDL11, 
WCL$^{+}$11, XCLZ19]. reaction
[XBSS19, YHG$^{+}$11, YJ11, Yu12a, ZYLL12, ZSZ$^{+}$14, ZX19, ZYR$^{+}$15, Zim13].
reaction-diffusion [RSLS13]. Reactions
[CC18c, ATP18, AAMD$^{+}$11, ABB$^{+}$12, ABB$^{+}$13, APA$^{+}$14, Cam15, CC18a, 
CSXZ17, Chu10, DSD$^{+}$11, DS12a, DGSVGM19, FB14a, FC16, FFA14, 
GAI14, GH10, GND$^{+}$12, GMBX$^{+}$16, GSMZ19, HLS12, HYUS11, HRL11, 
JZ17, JCG$^{+}$10, KG15, KZP$^{+}$18a, LLH14, LGW12, LT13, LXFC17, LJG$^{+}$11, 
MC10, MSV16, ORZ11, OSH17, RWR$^{+}$13, RB12, SBD$^{+}$19, ST13, Su10, 
SSX$^{+}$14, TM18, TN18, TXKT13, TTR$^{+}$12, Tsi17, UvSvdWK19, VKAM12, 
VKTR15, VGTL16, WHZ12, WCDM11, WSW19, XLY10, YZGS14a, 
YN17$^{+}$17, Yu12b, ZZI$^{+}$10b, ZZI$^{+}$10a, ZWZ11, ZLLL12, ZMW19, ZW17, 
dSLBNB17, dCRN18, dSVDM$^{+}$16, SMB18]. reactive
[DMAH15, HJLV16, IHJ$^{+}$13, LvDH13, MB14, NB19, RLLHL12, TDP$^{+}$12].
reactivities [WS11, WS12]. Reactivity
[FHG$^{+}$19, QQY$^{+}$18, TS14, WBKS19, BCP$^{+}$10, CRZ$^{+}$18, CBDS19, DI11,
S

[LLC17, MKH+13, NWW17, RGVC+19, SIG+11, WHK+12]. Robustness [VYM15, BD11]. ROCS [HP10a]. Role
[AS11, Cam19, CAD16, LPAS11, LLIW19, LJL+11, MCK17a, VL19, ZLX+19, ZT14, AALCM11, CFM+19, EJ13, GLF16, GFPSD17, HLBLCCG15, LeOdOldV17, OME16, PML+12, RF15, SGPSJ+17, SDB+16, SKMS13, SSA+17, VL17a, VMTL10, YDR13, ZRCC12]. roles

S


Semiempirical [FA18, SRL+15, BP18, GJK+19, GP11a, HGY15, KTN10, KB14b, LSD+10, MGWR12, Rez19, SPHI1, SDL14, TKNN10, TG12a, UCFR16, WCV15]. 

semiexperimental [VDVR14]. Seminumerical [PW12]. sense [DR14, ICS+12, ICS+13, NH19]. sensing [LZL+10, LCC18, RRK14]. 

Sensitivity [Han11, LL11, LWGW12, PDG+16, Sea10]. sensitized [ACS12, JYS+12, LZL+15a, MP19a, YJN+11]. sensitizer [YJN+11]. 

[SN16b, BLL13, BLG10, BRLS08, BRLS12, CC11, HS16b, KNP+12, LS11a, LCC+10, LYE+13, LZ18, LWL+10, Mat10, OAN15a, PML+12, PGdO+16, PHK14, PD11, Pog10, PFVL14, RLD12, SPS+12, Sch13, SWM10, SG10a, SG13, VLGK+17, VVGL+17, WX12, YOMT14, ZPP+16, FL15]. **Sets**

[TKN13, BLFZ13, BLBG+13, BLF14, BS10a, DBM+15, HSN14, Hili13, LOB18, LBH+11, LCW12, Leh15, Mit13, OLPB19, POB13, Sea10, SNKS10, STM+15, TH13, UCFR16, ZLT13]. **Setschenow** [XWW+11].

[TKN13, B LFZ13, B LBG+13, B LF14, BS10a, DBM+15, HSN14, Hil13, LOB18, LBH+11, LCW12, Leh15, Mit13, OLPB19, POB13, Sea10, SNKS10, STM+15, TH13, UCFR16, ZLT13]. **Setschenow** [XWW+11].

[AA18]. **seven** [PLAG11].

[AA18]. **seven** [PLAG11].

[AA18]. **seven** [PLAG11].

[AA18]. **seven** [PLAG11].

[AA18]. **seven** [PLAG11].

[AA18]. **seven** [PLAG11].

[AA18]. **seven** [PLAG11].

[AA18]. **seven** [PLAG11].
TN12, THP+15, VIT+15, XhD15]. silicon-doped [TN12].

**silicon-germanium** [GSMM15]. Silver [NSN19, Tsu19, YXZZ17]. silylene [BIL10]. **Similarities** [PM18a]. **Similarity** [HS12, LMZ+11b, YDL+10, CDM10, CDB10, CDBM11, CDC19, CQFC10, GWT+17, GK15b, HRK+10, HKS11, HS11, HSW+19, RMPAM15, TZCK18, YZZ16, ZYvIZ14].

Similarity/dissimilarity [YDL+10]. SIMONA [SWB+12]. Simple [Ano15-59, CNK97, GM17, MPSA17, AB16b, BS10b, BD12, CWZB10, KRTB10, NSP15, PHC13, PRIY+17, RHRCH16, RGVC+19, SEF+16, SS13c, YS18, dSAdSL13, KTSW11].


Simulating [HIS17, SS13c, FHT+15, PVM10, SA10]. Simulation [BVY+12, CRC13, Yan16, YKNN19, AASP18, AJA+19, AG11, AST+16, BEM14, BPPL12, Ber17, BLKP12, BFH+13, Bow16, CBP14, CLC11, CCW+10, CHKR10, CZNA11, DOM+11, EdOdS18, Fom13, FSC+14, GLZ17, GFGS18, GSD10, HM16, HYSF19, HQC16, HBJ+17, ISK14, IN19, Ish10, IM17, JA10, JJW+14, JAH+17, JSD+11, JCL+17, JWST10, JGS+17, Jor17, JP15, KV12, KVQC+11, KT18, KVR10, KAG+12, LL15, Lar12, Lar11, LWK+14, LJ+12, LCI7b, LMZ11a, LZ14, LWZ+19, LBDP12, MCVdV13, MSC+10, MBR+15, MTS+19, MSvG12, Mez10, MMZW14, MLCD11, MCC12, NPG17, NFG+13, NDD+10, OYK+11, ON14, PLZ17, PP19, QLKI19, RHNN10, RAR+11, RO14a, RO14b, RSR+12, RSLS13, SWM10, SK15b, SMRM+17, SSP19a, SHL19, SS19, SJZ+15, SBvG14, SAvG15, TNYN16, UTM11, UU12, VMRSH+17, Vor12, WC11, WLF19, WWW19, WSWD19, YAS13, ZX11].

simulation [ZSS+13, ZKH+10, ZLL+13, dCLFGL13, SGPI8]. Simulations [BRE16, Hes19, JL19, MFEM16, NN19, PK19, RJBH18, RKDM14, XFG+16, Aki16, BTA+13, BM12, BDTP11, BW15, BF17, BJJ15, BMBJ11, BB11c, BB11e, BCI11, CTR13, CCOH14, CVG14, CLK11, DGH11, DMN14, DSD+11, DHE+11, DZT11, DSK17, DLZ15, DDM+15, ER18, EK15, FTW12, GBL+11, GR11, GPM17, GCW14, GP11b, Has14, HCD+10, HFSO12, HPS12, HPKM14, HMM10, HYUS11, HJ10, HHWL17, HLEM18, II18, IPAA11, JS13, JWO15, JMS14, JND+19, KV13, KCK+17, KCK+15, KvdV14, KGKH12, KGHC15, KLOS10, KB11a, KTO11, KSR+16, KLS10, KMLS10, KZP+18a, KWL+16, KV15a, KPF+15, LH11, LCI7a, LRvdSM15, LZ12, LPS+13, LMI+14, LZLMP16, LCL+18, LM18b, LL19b, LAS+14, MPJ+19, MMH19, MN15, MCR17, MTvG12, MFEM15, MADWB11, MAP18, MKM+17, MB14, NST14, NFP13, NNK+16, NTNY15, Oht16, OC19].

simulations [OCL11, OLY17, OZ14, OCW+15, PGY15, PH17, PL19, PZCL16, PL14, PM13, PS13, PS10, PNG10, RD18, RdA12, RLG14, RSR15, SSO19, SBV10, SKA19, SS13b, SHFJ18, SBT17, SISK10, SCK18, SJ17, SMP17a, SYN+12, SK13, SFLG+17, SB15, SWB+12, SDMS13, SP+19, SV11, VSA11, VKTRJ15, VM11, WKL12, WAM17, WH11, WWKS11, WLC12, WBF17, WS19, WG14, Won18, WCJ+14, XFG+15, XWS13,
YKO$^{+11}$, YO$^{19}$, YSG$^{12}$, Yon$^{16}$, YHVM$^{12}$, YFH$^{+19}$, ZZY$^{+16}$, ZDKM$^{12}$]. simulator [BSL$^{11}$, KJM$^{+17}$, RLLHL$^{12}$, TCX$^{+13}$]. simultaneous [LL10b, WZWW$^{18}$]. Single [HPL$^{+18}$, LP11c, PM18b, SR18, Zim15, AS15a, BE14, BP18, BK17b, Den12, FTR15, GCCM15, KK17a, KGJZ19, LXL$^{+11}$, MSY19, MT19b, MCLD10, MEH18, PBE16, RHNN10, RLDJ17, SY16b, SPM$^{+19}$, TSR$^{+16}$, VS14, WLW$^{+10}$, WYL$^{+15}$, YZN$^{13}$]. single- [BE14]. single-bond [GCCM15]. single-configuration [MT19b]. Single-ended [Zim15]. single-excitation [MEH18]. single-file [SY16b]. single-ion [BP18]. Single-pass [SR18]. Single-sequence-based [HPL$^{+18}$]. single-step [RLDJ17]. single-vibronic-level [MCLD10]. single-wall [KGJZ19, TSR$^{+16}$]. single-walled [AS15a, PBE16, VS14, WYL$^{+15}$, YZN$^{13}$]. singles [EK17]. Singlelet [WNT$^{+19}$, SZL19, BSDP16, HWB19, ISO$^{+13}$, RS17a, SSC$^{+19}$, TCPPC14, ZZL19]. singlet-triplet [RS17a]. singlet/triplet [ZZL19]. singlet [NNT$^{+19}$, SZL19, BSDP16, HWB19, ISO$^{+13}$, RS17a, SSC$^{+19}$, TCPPC14, ZZL19]. singular [Les19, SG10a]. singular-value [Les19]. SiO [DOM$^{+11}$, HEM$^{+17}$]. SiOH [LvDH$^{13}$]. SIPs [KCC$^{+18}$]. Site [CH14, LJW$^{+11}$b, CVG14, DAP$^{+18}$, GEP$^{+14}$, GPD$^{+16}$, HL14, ISP$^{+10}$, LLB$^{+12}$, LKZM18, LLL$^{+12}$, MNNK10a, OHPR17, OHPR18, RLDJ17, SHF11, SB11, SC16b, TYN15, ZLX$^{+13}$]. Site-directed [CH14]. site-identification [RLDJ17]. sites [AIGP15, Ano12u, DVVP14, DBK17, JAH$^{+19}$, KDT$^{+12}$, LZTV10, LHL$^{+10}$, LL10b, LZ16, MA16, PHC13, PBG17, TYZ$^{+16}$, TYX$^{+18}$, Vor10, YZ15a, YHH$^{+13}$, ZZL$^{+12}$]. situ [JZL$^{+17}$, LZY12b]. size [DOM$^{+11}$, XhD15]. Size [NNT$^{+19}$, Tak18, AS15a, BLBG$^{+13}$, BD12, CC12a, CF14, DJX$^{+11}$b, FE14, G12, Hsu14, MTvG12, SL17, SB11, XYX17, Zha11]. Size-guided [Tak18]. size-modified [BD12]. sized [LRvE17, OGL10, RK15, WWD14]. sizes [Lin18]. SKATE [FM10]. slab [BBG$^{+18}$a]. Slater [Dil15, LRER13, MY17b, SFG$^{+17}$]. Slater-function-based [SFG$^{+17}$]. Slater-type [Dil15, MY17b]. slices [AKN16]. slicing [KCC$^{+18}$]. SLIM [SSBW14]. slit [Fom13]. slope [Zha12b]. Slowing [SGP18]. SM [XMSZ16]. SM-TF [XMSZ16]. Small [XYW$^{+14}$, ASS10, BTMS12, BLKP12, BS16b, CQFC10, DT19, DGL$^{+13}$, ETL17, GACAC$^{+14}$, GBFD12, KKPT11, KGHK12, KLJ$^{+17}$, KB11b, LK13, LHKS12, LH14b, Man19a, Man19b, MSS$^{+13}$, ME16, MBRC16, MPBJ11, NHH16, RLL$^{+10}$, RSSG18, RS13, SG13, STS15, TNY18, VT14, WF16, WTH$^{+16}$, XW15, XMSZ16, ZCGM11]. small-molecule [ETLS17, WF16]. smaller [MCK17b]. smallest [PMT16]. SMD [ALK$^{+15}$]. smeared [ENKK$^{+17}$]. SMILES [TTB$^{+10}$]. SMILES-based [TTB$^{+10}$]. Smoluchowski [KS18, SG10a]. smooth [AG11, EFS16, JLA17, ZSB$^{+16}$]. smoothed [LZ12]. SMOPS [XYX17]. Sn [MCK17b, PMG$^{+16}$, RDT14, YW12, ASS10, PKK17]. SnCl [dSDdAR10]. SnO [DHE$^{+12}$]. Sodium [KLN16, OC19, TFYO19]. Soft [SJC11, WBKS19, Ben17, BG12]. Soft-core [SJC11, BG12]. Software [AIGP15, Aki16, APK14, AAC$^{+16}$, BTA$^{+13}$, BHB12, BCSCJ$^{+13}$, BSZ$^{+12}$, Ber17, BIP15, BFH$^{+13}$, BBG$^{+18}$b, CBH14, CSEMB$^{+16}$, CZAF17, CAT$^{+13}$,
Software
[OPB⁺12, OZS⁺13, OC14, PSS14, PGL⁺15, PSG⁺17, PW12, PPM15, PHE⁺12, PVZ13, PG14, RLLHL12, RNSF⁺16, Rasz17, Réz16, RR14, RdA12, RSR⁺12, RCM⁺13b, SM14a, SFG⁺17, SK15b, SWA13, SMRM⁺17, She12, SC15, Si15, SJ17, SlvK18, SJL18, SWB⁺12, SDMS13, TNYN16, TSC⁺13, TTR⁺12, TTL⁺12, UU12, VMRSH⁺17, VVV⁺15b, VAR12, VBV13b, WdV12, WDY13, WPM⁺15, WF16, We12b, WHK⁺12, WHJ13, WG14, WCJ⁺14, XM11⁺15, XYX17, YY16, Yes12, Yes15, YHH⁺13, ZFOS19, ZDKM12, ZLL⁺13, dVAG16, CCC⁺11, DBF14, EdOdS18, FRC18, HSW⁺19, MSvG12, MJG⁺15, SF18, SBV10, SGM⁺13, Yal11, ZCS⁺15, She12].

Softwares [Ali11]. solar [ACS12, DGL⁺13, JYS⁺12, LZZ⁺15a, MP19a, SLC⁺17, TZ12, VAA14, YJN⁺11]. Solid [MP19b, RSK⁺15, ASS10, ASK18, CL16, HLS12, HBI⁺17, KLN12, KKH18, LOB18, OLPB19, POB13].

Solid-state [RSK⁺15, HBI⁺17, KLN12, KKH18, LOB18, OLPB19, POB13].

solids [BK11, BPC19, HAI⁺16, MDTD13, MS15, diRL11, Pon11, SN16a]. Solubility [MSY19, KKO⁺16, WZW18]. solubilization [TFYO19].

solute [BRLS08, BRLS12, EOA⁺11, RVM19, TKT11, YKO⁺11, Yan11].

solute/solvent [RVM19]. solutes [GC11, PAK15]. Solution [Cam19, PK19, AvKSP16, AK10, DR11, DBM⁺17, DP15, EOAO⁺11, GAI13, GAI14, HDK⁺12, HAL14, HNN⁺17, KS18, KTN10, KVR10, LvG10, MMB⁺17, FMM⁺12, PMC⁺17, PGG⁺17, SJ1E10, TKN10, UCF16, WHL⁺10, WC13, WLF19, XTG⁺11, ZLL⁺10, ZZ10, vADC⁺14]. solutions [Ber17, CFC15, EK15, Kri10, OC19, OCW⁺15, SM14a].

Solvation [Jia19, RNSF⁺16, ZBP11, ALRM18, CBG17, CBG16, FMG11, GMNH⁺16, GPK12, HRC13, JMLL13, JGS⁺17, Jor17, KSK11, LP11b, MS13, MPMA17, MBE16, NW17, OBW12, PL14, RK16a, RK16b, SM14a, SK12, SY11, SM15a, SM15b, SMM⁺18, TKYN17, TCC⁺13, WXL17, WWW18, YMT14, YAS13, Yan14, ZCS⁺15]. solvation-free-energy [SM15a, SM15b]. solvational [FCL⁺10]. Solvatochromic [MKH15].

Solvatochromism [TKYN17]. solve [PNW⁺16]. Solved [CD19]. Solvent [KC13b, PK19, AKK⁺16, BEM14, BRLS08, BRLS12, CAD16, CBG16, EK15, FYZ⁺12, FDI6, GA19, HDL⁺17, Has14, HPL⁺18, HYUS11, KJDB12, KB11b, KCPM12, LHL⁺10, LC17b, LZZ⁺16, LWZ⁺17, MBC11, MBC13, MS11, ML14, MCUJ15, MCG12, MNNK10a, MNNK10b, PDMM10, PS13, QY⁺18,
RVM19, RdA12, RRK16, SLT14, SBV10, SK17, SLX+15, SYH12, SCMA+17, SKMS13, TYN15, WWKS11, WXL+12, WBF17, YOMT14, Yan14, YJ11, BK17a. solvent-dependent [HYUS11]. Solvent-driven [KC13b].
solvent-induced [AKK+16]. Solvents
[LHT15, ISO+13, Pie14, Pog10, RK16a, RK16b]. solver
[FBY+17, FHMB15, Kan15, RR19, SHF11]. solvers
[GRARO+14, WL10, XYX17]. Solving
[KV13, SG10a, BYE+16, GA14, RRFV+18, SK15a]. solvolysis [OSS10].
SOMA [BMFG16]. Some
[RCM+13b, CME11, CC18a, CCYL11, CXS10, MJLV14b, Vyb16, ZPF14]. sometimes [VDVR14]. Song
[JW12].
Soon
[Ano16-75, Ano16-80, Ano16-81, Ano16-82, Ano16-83, Ano16-84, Ano16-85, Ano16-86, Ano16-87, Ano16-88, Ano16-76, Ano16-77, Ano16-78, Ano16-79].
soot [KAR12]. SOP [AKK+16]. SOP-GPU [AKK+16]. Sorafenib
[GMASBF16]. sorbates [KB19]. Sorting
[NMF+14]. Source
[GMBM18, TCB16, Aki6, APK14, BZH14, CD13, FBY+17, HMO+18, HLS+13, HPT17, KSD+12, MLG18, PHT17, SMRM+17, XTG+11, Yap11, Yes12].
Source-Function [GMBM18]. sources [BK13]. Space
[vRWGS17, ACD+13a, ACD+13b, AD10, Cas13, CH16, CXS10, Coh18, DK11, DSHLM18, FC18, GA14, GKA5b, HB14, HP10b, HSB+11, JCGVPHT17, LMZ11a, LLFH16, LAW+16, MBFP15, NH19, NCT18, PDG+16, SS13a, SHL+11, SCSW13, TNT19, TJB12, WDHZ13, XTn18, YD17]. space-group
[HB14]. spacer [JYS+12]. spaces [CD13, FBvdB18, TNT19, WM17].
spanning [yOaCG10]. sparse [LK11, LDH+14, VZ14, YHH+13]. sparsely
[CBP+15]. Sparsity [HNS16, BYE+16, RR11]. sparsity-exploiting
[BYE+16]. Sparsity-weighted [HNS16]. Spatial
[PTB+15, HAL14, MTvG12]. SPC [GM17]. SPC/E [GM17]. SPC/E-I
[GM17]. special [Alg17, ZZ19]. species [MAK+14, MG11, OSS10, RHT+15, SSA+17, TCPPC14, Tsi14, VRKT19, WvRSM14, ZZ10, ZLY+16].
Specific
[DHF+11, OHNK11, CIKT13, CCM15, GCCM15, HNyH19, HYM16, JZZM14, KR12, LHO17, LGL11, LFHC17, MCC11, MC12, SSSM15].
specificity [LJW+11b, LBS10, ZX11]. Spectra
[PAK15, TT18, AMQ+14, BG17, DCOD13, EBPK17b, FD13, FF11, GWF11, GGM+12, GZZ12, HHH+17, KASH14, Kow11, LBC+12, LK11, MAK+14, MCLD10, MKK+19, NHF+10, PMC+17, PDMT10, PDG+16, RS17a, RJS17, SGT10, SB15, SR11, TYN15, TZCK18, TG12b, Tsi14, WGL12, WWD14].
spectral [Ano15-58, BH14, CBDS19, HRMAL+13, KZZ+16, NSO+14, QZM11, RLG11, SFDE16]. spectrometer [LBB+15]. Spectroscopic
[SS13b, GK10, KDB13, KOP15b, NC13, NC14, TCPPC14, TSI14, ZLL+10]. spectroscopy [DMD+18, HDM+19, HPSK12, IY18, KINR+18, LLO12, Lin18, NC12, OC19, WHK+12, FAS+18]. spectroscopy-oriented [HPSK12].
spectrum
[BLF14, KCC+18, MN19, MLCD11, RDF+11, SLL13, TSC+13, ZDX11].
state-of-the-art [YJ19]. state-selected [KCL+14]. State-specific
[CCM15, GCCM15, LGL11, LXFC17, MCC11, MC12]. state-to-state
[XCLZ19]. States [GBMB18, AST+16, ANH+11, BSL+16, BH19, DHOG13,
DSV+19, EFS16, EK17, EVR18, EP15, FAA15, FD16, GO13, GA12, GTK10,
HDHL15a, HDHL15b, HDHL15c, JCGVPHT17, KKH19, KT19, KKA+18,
KPG18, KB14b, LLBO12, LLW12, LWW12, LGC19, LX11, LS11b, LYSS11,
LCK+18, MS10, MN15, MGCC19, MH11, MEH18, PBDW11, RHRCH16,
SRF+17, SSC+19, SOYC12, SM†+19, SB13, SB15, SZZS16, TN10, Tia12,
TSN17, VVV+15a, XWSW13, YZGS14b, YK13, YLZ+10, YB11, ZXS+10,
ZBB16, ZDT18, dLC17]. Static
[KBC12, BS10a, KZK+12, Lu11, PC14, PNW+16, PM13, WYT17]. Statics
[Pon10]. stationary [BHR15, Can10, Can11, LHMM11, SLT14]. stationary-point
[BHR15]. stationary-wave [Can10, Can11, LHMM11]. Statistical
[JHH+13, PZA15, PTB+15, FL15, GZ14, HMYZ16, ICS+12,
ICS+13, Kan15, KMLS10, PTK11, RB13a]. statistically [GR10a, GR11]. statistics
[QZ10c]. steepest [MS16]. steepest-descent [MS16]. Steered
[Won18, FBEM11, KERY+16, MJC14, NFG+13, SJ17, WTD+19]. step
[AYYO17, DS12b, DGC14, GRCL12, JWO15, JS17b, KvdV14, LLvG10,
LGL11, LvG13a, LL10c, RLDJ17, RS12, SJC11, TCPPC14]. steps
[REH13, Zin13]. Stepwise [DLP11, LZ18, GRCL12, ZL11]. stereochemical
[WCDM11]. stereochemistry [PPJ14]. stereochemistry-dependent
[PP14], stereodynamics [Chn10, CSMN+18, LWD13]. stereoelectronic
[AS11]. Stereoselection [BJSI2]. Steric
[RMGB11, MJLV14b, MP17a, YNH+17]. sterically [MH17]. Stern [MBA11].
stereoelectronic [HLBCCG15]. Stevens [BCJC+14]. sticks [CVT+11].
stilbene [BW11b]. stk [TBJ18]. Stochastic
[AFPI13, CGP12, ITY+19, AC12, ESD18, KV12, KV13, MS16, MCP18,
NC13, PH17, RSL13, SWB+12, VBD11]. STOCK [BPJ15]. stockholder
[FHZK+18]. stoichiometric [VI17]. stoichiometry [FSD+18]. Stone
[DWZ+17, YNZ13]. stool [FPB12, FB14b, ZCK+16]. storage
[BE14, BEPM14, DLT17, WKL12]. Story [Sce07, Sch10]. Strain
[DM15, FB12, FC16, FLM11, JWO15, LSL+19, PBE16, She12, SHL+13,
strategies [AFBR17, BSDP16, cCVG+14, DSX+11, LT16, Rao11, SCOJ13].
Strategy
[Jia19, CLX+10, C2NA11, HJKJ13, KTN10, KKH18, LLL+10, PHC13, PH17,
RVVK13, SHL19, TKNN10, WO15, XHLH16, YDGZ15, ZGZC19, SMD18].
StreaMD [DJS+18]. Strength
[ELKE19, JLLW19, Fra15, Fra16, KSC16, LGKS17, MPSG11, YJ17, YHW17].
strengthening [MS11, LYS11]. strengths [CKL+11, MLC13].
streptavidin [MLZZ12, ZJZM13]. streptavidin-biotin [MLZZ12].
streptocyanines [WYT17, XKW18]. Stress
[BS19, GMBX+16, HXM+16, JMX+16, NI15, NFI+16, XFX+16]. stretch
[CK10, RS17b]. stretching [KLS10, KMLS10, TKCN19, dSH19]. string
BMFG16, JZ17, Zim15]. **stringent** [DPOS16]. **strong**
[Kan15, MLZZ12, SDF12, SS19, VVY17, Vik11, ZSL17]. **stronger** [KSC16]. **Structural** [ESD18, FHG+19, GLF16, GBL+11, GTT10, GAMAC+14,
GWX+12, HS17a, II10, KZK+12, KSD+12, LBT11, MP19b, NC14, TS11,
V SH19, ZWW10, AIGP15, AD10, AKK+16, ALH+10, BOBO16, BPC13,
CD19, CPV+12, CDS16, CYI+10, DUL11, DH11, GWT+17, GNI18, HS17b,
HVS16, KPK11, KG11, KNE11a, KDT+12, LL13a, MCF10, OSA19,
PHA13, PGY15, PNG10, RKF11, RKB+14, RSL16, SFA17, SS13c, TYX+18,
VVW+18, WC11, XMSZ16, YVEI+17, ZWW10, FAS+18, VPR10]. **structurally** [TZCK18].
**Structure** [BPPS19, BJP15, CGBK13, DXL+10, GPK+16, GWJJ12, GBGR16, HLB15,
JLLW19, LAHS16, MM19, MHR11, NC12, NC13, PMG+16, Rab12, SGH+16,
VDVR14, WZK+13, AFPI13, AR15, AM19a, AM19b, AJR16, AC12, BPPS17,
BFH+13, BD13, CPRS18, CD13, CV19, CM13b, Clo15, DKE+17, DK13,
DSB+19, DDP16, DVVP14, DGSVGVM19, DLW12, EH13, EK+13,
EFOD13, FZY+12, FD19, FSC+14, GLB16, GMSdG15, GRARO+14, GP12,
GK10, GRD+10, GPDc+16, GBG+19, HASR+12, HNH13, HS17b,
HNYH19, HS14a, HRB+17, HH15, HMYZ16, HZ13, HLW15, Hua16, Ibr17,
KYT+17, KKH19, KSM17, KT10, KS12, Kop19b, KKL+13, KLS10, KMD10,
LBO12, LFB14, LKL10, L+11, LMI+14, LYL16, LPE+10, LGL11,
LH11, LWG12, LLFH16, Mat10, MDT10, Mau14, MAPB10, MV17,
NGAS17, NCT18, OCL11, OL13, OLA15, PSS14, PdSC18, PLM+12].
**structure** [PN13, RLG14, RCM+13b, RR11, SHMO11, SB10, SM11,
SLP+12, SB19, SLIB12, SRS14, SYN+12, SKGB13, SPZP18a, SPZP18b,
Tacl9, TN12, TT+11, TG12b, UNT16, VV12, VHR16, VVBL17, VA14,
VBM13, VKC10, VI17, VLGK+17, WO15, WGN11, YY12,
YZ16, ZRCC11, ZH11, CPR18, FDCJG18, OFS12, SA10]. **structure-activity** [DXL+10]. **Structure-based** [CGBK13, DXL+10, DVVP14, GLB16, VKC10, YZZ16]. **structured**
**structure** [GEP+14]. **Structures**
[DLT17, HDM+19, NSN19, SNS16, SZL19, ZLX+19, AHK+19, BHKS14,
BPM15, Ber17, CL16, CC14, CBDS19, CV12, DVVP14, DH14, DCM18b,
DT19, DZA11, GS12, GSS13, HSY+11, HTS17, HPL+18, HS12, Hua16,
IK10, KNE11a, KOY+12, KTO11, KTO13, KDT+12, KSW16, LABSG17,
uLH111, LXZ+10, LLW14, LL19b, LAc14, MGS11, MTM14, MPA10,
MPA12, MP13, Mau14, MN19, MH10, MCAY15, MP17b, NS18, PRP15,
PNW+16, QZM11, RHR16, RAO11, RCR+16, RV11, RHJ11, RVV13,
RSG+10, Sak18, SWA13, SFR+11, SJ11, SIT18, SPM+19, SKY+11, TN10,
Tak11, TFO+10, TFO+11, Tsu19, UCF16, WKC11, WD10, YNH+17,
ZSL+11, ZLY+16, ZP13, CM13, OSI+19, PGCT+12]. **studied**
[Ish10, KRTH10, OLY17, RHPWS13, RI10, TS15b]. **Studies**
[JM12, AALCM11, BLS10, BRSN12, BLG10, BIL10, DM15, DXL+10,
FWS+18, GZZM16, GEP+14, JLS+10, KG15, KP11, LFC17, LCW10,
LJ+11, LWD13, RCM+13b, SB10, SFA17, SLHW09, SZZ+18, TNI+19a,
substituents [CBTZ16]. substituted
[AARP17, BEPM14, CCCLRO14, CZH12, DCHL12, KYCL11, KV15b, LZH16, LWL+11, LTP11, Lu11, OSF12, PRRT+10, QCR12, SSP+13, SK12, SKGB13, UT14, WGL12, YPC+10, ZZWT12]. Substitution
[MUN+19, CFM+19, ITY+19, LGW12, MPSG11, TZ12]. substitutionally
[VS14]. substrate [AALCM11, BHNS14, BEL+11, JDW+19, LZL+16, VCM15, WWW19, YZLZ18]. substrate-binding [WWW19].
substrate-enzyme [BHNS14]. substrates [QQY+18, Tsi17]. substructural [PSdPE+10]. subsystem [SFG+17, UDK+18]. subsystems [DK11, PL14].
subtilis [CPK12]. Subtraction [Hes19]. sugar [JSD+11]. suggested
[GZL+12]. Suitability [BVHI17]. suitable [TZ12]. suite
[DMN15, PGL+15, FPVI3, LJC+19]. suited [EK17]. sulfate
[CHKR10, PP19, TFYO19, YZGS14a]. sulfide [LW+16, ZYG+14]. sulfides
[OSF12]. sulfonyl [YHVM12]. sulfonyl-containing [YHVM12]. sulfoxide
[GC11, KPH+19]. sulfur [CTR13, HS+14, HS16b, Kop17b, OSF12, WGL12, WZC+19, YB11, ZM10]. sulfur-containing [DT19, ZM10].
sulfurization [TR12]. sum [SB13, SB15, Tak14, Tia12]. sum-over-states
[SB13, Tia12]. sumanene [CLFRO18, CBTZ16]. summation
[GBDF12, SF18]. summations [SB13]. super
[CBB11, SF18]. superfraction [CSSB11]. Superacid [KS19].
superacids [EHSPT16]. superalkali [LLD17]. superatom [LYL16].
supercharger [FRN15, RFN15]. Supercluster [Hes19]. supercomputers
[KNHN16, KN17]. Superhalogen [KS19]. superlattices [KC13b].
supermolecule [XZ1]. superoxide [GEP+14, CPR18]. superoxo
[ZRC+12]. superposition [CDMB11, HS12, PD11, YLGX14].
superpositions [Kne11b, LAT10, LAT11]. Supersecondary [ZHHX11].
Supersites [Hes19]. supertetrahedral [GKB+19]. supervised [DGPM14].
support [GTZ+18, HJ13, RLL+10, RMRBH+19, Sie18, TYZ+16].
supported [CZZL19, SN16a]. supramolecular
[CSGOA17, HLBI5, OAN15b, SMDP18, TBJ18]. Surface
[Hes19, LLW19, LKI6a, SRS14, Ano15-58, BPM15, BH14, CM13a, CR14, Che17, CZZL19, DBM+15, DS12b, FZY+12, FMNC11, FVP14, FDH19, GCWS15, GY10, HLVdV13, HTY19, HWLW11, HYD10, IN19, JZ17, JX10, KT19, KKR+13, KTSW11, Kop16, Kop17a, Kop17b, Kop18, LLH14, LL13a, LYC+13, LWZ+17, MK13b, MA+14, MB14, MOS12, NW17, OKIS17, OHPR17, OHPR18, PZAI5, SRSL015, SAKAI9, SH14, SBC+11, SLG15, SLL13, SIG+15, TSR+16, WXL+12, WXL17, WBF17, XFX+16, XCLZ19, YPD13, Yan14, ZLT13, ZKE+17, MK11]. Surface-enhanced [SLLL13].
surface-supported [CZZL19]. Surfaces
[BHB19, ZQH19, AKN16, BPC19, BHB+17, BS16b, CCJ+11, CSXX17, CZNA11, GFG11, Hei10, HRL11, IN13, KIOY19, KLS10, KMLS10, LX11, LAW+16, MCC11, MSC+10, MCF10, MK19, NPP13, OHPR18, Pol13, RNSF+16, RRC+15, RBOH11, RLA18, SRF+17, SFR+11, SC15, SFLG+17, TG12a, VT14, VVY18, WKC+10b, YZ15a, YR13, OSI+19]. surfactant
Taurine [YW13]. tautomer [WHJH13]. tautomeric [SJWE10].
tautomerism [BMB13, LGOM+15, SC18b]. tautomerization
[BH13, BZH14]. tautomers [BZH14, dALdS+15]. taxadiene
[EvRC+18, vRET19]. Tb [SRL+15]. TD [HL19, TS15b, CCB15, CH10,
DSB+19, EFA13, HRJ+14, HRJ+15, HL19, JRSHP14, KKL+13, KP10,
LZL+10, LZHH11, LSH+11, LYSS11, RDF+11, SRF+17, SCF+19]. TD-DFT
[CCB15, CH10, DSB+19, EFA13, HRJ+15, HL19, JRSHP14, KKL+13,
KP10, LZHH11, LXZ+10, LYSS11, RDF+11, SRF+17, SCF+19]. TD-DFT-
[LSH+11]. TD-HF-based [LSH+11]. TDDFT
[SFCck+15, CMF+17, LRBB12, MS11, QCR12, SFCCK+14]. Te
[AM19a, AM19b, PLFS18, SPS+12, HSJ18]. technique
[AMGB10, BG17, LZL+13, SMM17, TSR+16, TTn19]. techniques
[BCP+10, BCG10, GVP+10, MCP18, RD18, SDF+17, SPL+18, SY11, WBN+13].
Teller [BMD19]. tellurium [RRK16, ZWGO16].
Temperature [HS17b, HYNS19, KKO+16, LPTc12, PBE16, SY16b, SMM+18,
ZQH19, CH16, DKT13, DLSD13, HDM+19, KCK+17, LL11, MK17, MKK+19,
OGL10, TldG+12, TM16, VED10, WMW11, WWT19, YW12, OCW+15].
Temperature-pressure [HYNS19]. Temperature-shuffled [HS17b].
temperature/Hamiltonian [KCK+17]. temperatures
[NMLD13, RHNN10]. tempering
[GC18, LAW+16, MO15, MO17, NPTS16, TKT11]. Template
[LI19, Man14, GLF16, KCK+17, ME10, YHH+13]. Template-Based [LI19].
Template-free [Man14, YHH+13]. template-restrained [KCK+17].
tension [NFPD13]. tensor
[BS19, CPZ19, Elk16, EWK+13, GMBX+16, HXm+16, JMX+16, KK17a,
NFPD13, NIIT15, NFI+16, TKC+11, XFX+16, YA018]. tensors
[EPD+11, PHK14]. tepidum [KPG18]. terahertz [KB16]. term
d[SFs17, JBsg11]. terminal [MK+16, YXZz17]. terminally
[KLs10, KMLS10]. terminally-blocked [KLs10, KMLS10]. Terminated
[BHP19]. terms [BSA14, Czy11, CWZB10, RRH12]. ternary [RDT14].
tertiary [Opr16, SM11]. tessellation [MOs12]. Test
[PHC13, BS10b, DSB+19, DPOS16, WOn18]. tested [HMM10]. Testing
[Gil11, II18, MPSA17, RLD12, JGS+17]. tests
Tetra [BHP19, WDLG12]. Tetra-Anionic [BHP19]. tetraamines
[SB10]. tetracarboxylates [CRC13]. tetracoordinate
[XHd15, ZYW+16, ZLY+16]. tetraene [ABDGN12]. tetragonal [LKZz18]. Tetrahedral
[LBC+19]. tetramer [Ish10]. tetramers [LYL16, ZZS16]. Tetraoxide
[JW12, SLHW09]. tetraprotonated [ZYW+10b]. tetradical
[Cas14, YSSB12], tetrascarhide [NPG17]. tetrahiafulvalene [MCF10].
Tetrazine [JW12, MCAG+16, SLHW09]. Tetrazino [JW12, SLHW09].
Tetrazino-Tetrazine-Tetraoxide [JW12, SLHW09]. tetetel [YKH15].
tetroxide [MCAG+16]. text [HRKS11, HS11]. text-based [HRKS11, HS11].
TF [XMSZ16]. TGMin [CZZL19]. Th [MCK17a]. ThCl [LCL+18]. their
[ARRC15, Ano11, AM19a, BSG18a, CC12a, CBTZ16, CFC15, CB11a, DLT17, DSM+11, GPM17, HJ13, JMLL13, JHMB+09, JHMB+11, KG15, KNE11a, KRSC12, NYH+17, SBR13, TN12, Tak11, TY10, TS11, VV15, VVV17, VVBL17, XDL+10, ZWY+10a, GMBM18]. them [WCWV15]. theorem [CDB10, KSH13, YB16, ZM11]. theoretic [CRZ+18, MCC12, ZLW10].

Theoretical

[AvKSP16, AMAA+11, AWF+18, AHK+19, BHB+17, BSDP16, CWT+12, DBM+17, DGL+13, FF11, FWS+18, GYX+10, GLZ17, GLM+17, HW19, HDHL15c, JW12, KCB+12, KSO+19, KMT+19, KS13b, LCL+10, LWL+11, LW12, LZY+12a, Lin18, LWG12, LX16, LXFC17, LD18, LGJ+11, MLQ+12, MSV16, NSN19, NFI+16, OSS10, OAN15b, PPK17, PM13, PE11, RS17b, SB10, SMN+19, SSD19, SKY+11, STS+10, SSZ16, SLC+17, SGL13, TPL+10, Tsu19, WMW11, WHDL11, WCL+11, WS12, XBS19, YJN+11, YPC+10, YHG+11, YCGA10, YYT12, YDGZ15, ZZL+10b, ZZL+10a, ZYLL12, ZLL12, ZSZ+14, ZYG+15, ZGZ19, ZBMZ15, dSdLBNB17, BLS10, BAD+19, BE16, CZH12, CKL+11, CBTZ16, EV14, GG10, HDB15, HGP14, LW12, LDL17, LZW+11, LCL+18, MRC+18, MPSG11, MP19a, MKK+19, NFF+10, NJX+10, PH12, PdSC18, PdSP+10, Pog10, PH10b, RZG+13, RVCF13, RVP+13, SSP+13, SSC+19, SJD11, SLHW09].

theoretical [SKT11, SGH+16, Tak11, TL16, UCRL18, WSH10, WQ10, YK13, YW11, YZ13, YZ13, YD10, Zha12b, dSdSL13, HDHL15a, HDHL15b, KZK+12, TDP+12]. Theoretically [LLX+19]. theories [OM12, WCWV15].

Theory [BHB19, CKH19, EV18, ELKE19, GNC+18, IUK+11, LLX+19, MP19b, Sah18, SXZ13a, SXZ13b, WBKS19, WM12, AMK11, ALK+15, AR10, Ali18, ARAG17, ABDGN12, AW19, AG12, ASS10, BY11, BLDG+13, BS19, BMD19, BZB+13, BG13, CHG+16, CRZ+18, CSAdOM17, CWHH11, CKH17, CCM15, CF14, CC11, DAP+18, DCHL12, FRSA14, FD16, GHL17, GZL+12, GCCM15, GWW19, GLW19, GY10, GNGCA10, GND+12, GA18, GEG11, GPA12, Han11, HPT17, H113, HNN+17, HRJ+14, HRJ+15, HG10, ISN13, IKN13, IM17, JRSPH14, JHL+14, JW16, JYS+12, KHBW17, KLN12, KML13, LCW12, LBGS16, LCL+10, LLH17, LPMT17, MCC11, MHH19, MAK+14, MWJ+11, ME10, NPG+18, NMLD13, NO16, Niz13, ORZ11, OZLSBH12, PAK17, PML+12, PPH+14, Pie14, Fyy13, QZ10b, QZ10c, QB16, RAGL11, RJP12, RCM+13a, RML+15, RB12, RSLML12]. theory [RHPWS13, RNS19, RR19, Rui11, SM14a, SFG+17, SHL+18, SCW11, SSSM15, SHF11, SEF+16, SE14, SH14, ST13, SHL+13, SSMW09, SB14, SM+18, SKT11, SZ16, STS15, TdG+12, TAG16, UvSdWK19, VDL+13, VVP12, VV14, VL17a, VAMS14, WHL+10, WDLG12, WHX+10, WQ15, WL14, WGN+16, XTY+14, XYW+14, YJ11, YLZ+10, YS13, YKH15, ZXS+10, ZSWL12, ZL14, ZDX11, ZYG+14, ZWY+10b, ZYW+10a, ZLHH14, dSdS12a, dSdS12b, vLBBR12, FAS+18]. theory-based [YJ11].

theory/configuration [HPT17]. theory/time [JYS+12].

theory/time-dependent [JYS+12]. therapeutic [AFBR17].

theory [ZZ12]. there [MLGB16, Sie18]. Thermal
[LL10c, SJSS19, ASL+11, BIL10, NGAS17, OZLSBH12, VVW+18].
thermally [FWS+18, IHY15, ZGZ19]. thermocalc [HDH12].
Thermochemical [TFQ+11, KSM16, TN12, WDW12]. thermochemistry
[HDH12, Sán17, SB14, TCGNT18, VRKT19]. Thermochromatium
[KPG18]. Thermodynamic
[EOO+16, NSK18, PAT+10, BE12, BPE16, BB11b, BB11c, CBH14, CC18a,
EBPK17b, HIL+17, Hug12, MMB+17, PGY15, PBE16, RNSF+16, RRF11,
RKB+14, SS13c, SJIC11, SJ16, WC11, dRBO13]. Thermodynamics
[DS12a, RS12, BRE12, DMJ17, EHSPT16, HRC13, Kan15, WRM+12, ZYL+12].
thermoelectric [KLZ+18, NGAS17, YW12]. thermolysin
[DHF+11]. thermometer [SPZP19]. thermophilus [TNI19b].
thermostat [JWO15]. thermostatization [PH17].
Thermus [TNI19b]. thia [GMASBF16]. thia-calix [GMASBF16]. thiaphosphiranes
[ZSLL17]. thiazol [BMB13]. thiazol-2-amine [BMB13]. thienylenevinylene
[TZ12]. thioacetamide [LCB10]. thioamide [KG11]. thioformaldehydes
Thiophene [PH10b, PRRT+10, YHCS11, ZSTRS+18, ZSLL17]. thiophene-based
[ZSLL17]. thiophenes [Su10]. thiophenic [NHF+10]. thiophenol
[AMAA+11]. Thiophenols [CGVBAI19]. thiotropolone [DL19]. thiourea
[TKN13]. Thole [AS15b]. Thomas [Spr10]. thorium [KKH19]. those
[SIG+15]. ThQs [ZZL19]. ThQs-C [ZZL19]. threading [Mau14]. Three
[CKH19, NR11, NF17, NNK+16, TYN15, TKC+11, CXD+19, HJKJ13,
KYT+17, KRSC12, LYSS11, LK16b, MBT14, MS16, RVM19, SLT+15,
TDKT10, TTX+13, UT15, WC14, YLL11, ZZL+12, ZWX16]. Three-body
[NF17, RVM19]. three-center [CXD+19, YLL11]. Three-dimensional
[TYN15, TKC+11, KTY+17, KRSC12, TTX+13, ZWX16]. three-domain
[MBT14]. three-level [HJKJ13]. three-membered [TDKT10].
Three-Range [CKH19]. Three-residue [NR11]. threshold [LCM16].
through-put [GKJ+19]. through-put [ESB13, JBAM11, PVJ10, RNS19].
thymine [HvM12, LJJW11a, ŠBD+17]. thymine/thymine [HvM12]. Ti
[MP19b, WWKS16, WZH+18, YW12, BH15, SDB+16]. Tian [Aneol2u]. Tide
[RB12]. Tight [Lar12, NN19, YKKN19, GAJ+17, HNWF07, HNWF12,
JCP14, KZZ+16, MSY19, MAP18, MFR+17, NF17, NN18, NO16, NKK+16,
Oht16, Res19, SPS+12, VHS+19]. Tight-Binding
[NN19, YKKN19, Lar12, HNWF07, HNWF12, JCP14, KZZ+16, MFR+17,
NF17, NN18, NO16, NKK+16, Oht16, Res19, SPS+12]. tightly [PG19].
Time [GTK10, KS18, PAK17, WHL+10, WHX+10, YLZ+10, YKKN19,
ZDX11, AYYO17, CHG+16, DGC14, Fom11, FSSW17, HCD+10, HNWF07,
HNWF12, HIL10, JWO15, LS17b, KNR+18, LL13a, PNG10, RS12,
RHPWS13, REL17, VHR16, VIK11, ZXS+10]. time-averaged [HCD+10].
Time-Dependent
[YKNN19, GTK10, KS18, PAK17, WHL+10, WHX+10, YLZ+10, ZDX11,
timescales [MCR17], time-step [AYO17], times [VBDS11].

Tinker [HLW17], TiO [NC14, TSK12, CCJ11, DSB19, EP15, HRL11, MP19a]. TIP3P [SA10].

TIs [BE14, RSKG14]. Titan [OZLSBH12]. titanium [QZ10b]. titration [HS14b].

TMBiM [LWXC16]. TmoleX [STH10]. TMS [YXZZ17].


Tool [LH19, BPC19, GKJ19, HKR10, HKS11, HS11, HG13, JLS18, KDB13, LP11a, LK11, LDB17, LCA17, LBB15, LG11, LP11c, MTD16, MCC12, NHK13, OV14, OVPK15, OC14, PNW16, SDMS13, SH19b, WCDM11, ZCGM11, dVAG16, JCGM18].

toolbox [HPT16b]. toolchain [KSH17]. toolkit [FSC14, GS12, IGK16, MJBM12, MSS13, MADWB11, NKJ16, PG15, PPM15, TS10a, TBJ18, ZLL13].

Tools [RLG14, ZFOS19, GMZ12, SLG15].

Topo [BGL18]. TopoG [KYG15]. Topographical [KYG15]. Topography [PK19].

Topological [Jan16, AR15, BGL18, PRY17, Pop18, SB11, TSQ12, Tan19, VAR12, VBMA13, Wei12b, vSGP10].

Topologies [Gar12, TSNC17].

topology [AD10, ASS17, Dill15, FED17, GMSdG15, KP11, MSCP17, yOACG10, Rod13, dCDP15, BLG10].

Topomerization [GG10].

toroidal [SS13b].

Torque [Elk16].

torquoselectivity [GMBX16].

torsion [DSPL16, FZY12, HP10b, HXM16, JMX16, YZ16].

torsional [VL19, BAS14, PRRT10].

torture [RHT15, ENKK17].

torus [WRG17].

total [BEEL14, IKN13, MA16, SM16a, WX12].

toxicity [TTB11, TTL12].

tQ1 [VL17b].

tQ1/PC [VL17b].

track [ENKK17, RHT15].

tracking [BHR15, GBPC19].

tractability [KFY13].

training [DBDP16].

trajectories [AST16, HRD16, JZL17, KG13, LZS17, PSP15, RN17, SKA19, SFR11, ZSS13, dSdM16].

trajectory [UK11, JJW14, LW13, LAS14, MKS12, PVZ13, RC18, SBD17, Yu12a].

Trans [CSM16, MSBF16, Tsi19, WS19, BLS10].

Trans-2-Butene [CSM16].

Trans-effect [Tsi19].

trans-influence [Tsi19].

trans-influence/trans-effect [Tsi19].

Trans-philicity [Tsi19].

trans-pinane [BLS10].

transcription [XMSZ16].

transfer [Alg17, AK10, ANH11, BHB12, CMF17, CSAOM17, CPLL11, DWR17, DAdGR15, EFAC13, ENKK17, FC16, HSH15, HAP12, HDHL15a, HDHL15b, HDHL15c, IYK11, JM11, JGVPHT17, KGR16, KDR18, LZL10, LLL11, LWGZ15, LPB16, MPSG11, MRB14, MSV16, MCF18, MT19b, PGCT12, PG18, PAK17, PL14, PTB15, Ras17, RCM13a, RML15, Ric16, REL17, RKDM14, SRF17, SBD17, SMP17a, SZB19, SHB17, TM16, Tsi17, VKTRJ15, VMTL10, VL17b, WCT11, WZ19, WG14, XBS19, XLY12, YKH10, YHX19, YLZ10, YYT12, YFH19, ZW17, dALDS15].

Transferability [FP17a, ZRL15, HOK17].

Transferable [EKH14, VVLG17].

transforms [YZSG14a].

transform

[Ano15-58, BH14, Ish12, LL13a, SZZT10, IY18, NZM18, YW16].
transformations [HDL+14, Min18, SJC11]. Transiting [CM13a]. Transition [BF19a, BGS+19, ZQ10c, YB13, Alg17, AR10, BS15, CSA10M17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JZ17, JSF19, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, MKK+19, NMLD13, PHK14, RAGL11, RIJ+11, SJZ+15, VV+15a, VHS+19, YZG14b, YWZ14, ZWW10, Zim15]. transition-metal [LDZW17]. transition-state [CSA10M17, RAGL11]. transitions [AKK+16, BD11, DH11, HS17b, HB15, KIYO19, MCvdV13, PBDW11, SBT17, SPZ18a]. translationally [MRO17, MK19]. translocation [BF19a, BGS+19, OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JSF19, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, MKK+19, NMLD13, PHK14, RAGL11, RIJ+11, SJZ+15, VV+15a, VHS+19, YZG14b, YWZ14, ZWW10, Zim15]. translationally [MRO17, MK19]. translocation [BF19a, BGS+19, OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JSF19, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, MKK+19, NMLD13, PHK14, RAGL11, RIJ+11, SJZ+15, VV+15a, VHS+19, YZG14b, YWZ14, ZWW10, Zim15]. translationally [MRO17, MK19]. translocation [BF19a, BGS+19, OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JSF19, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, MKK+19, NMLD13, PHK14, RAGL11, RIJ+11, SJZ+15, VV+15a, VHS+19, YZG14b, YWZ14, ZWW10, Zim15]. translationally [MRO17, MK19]. translocation [BF19a, BGS+19, OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JSF19, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, MKK+19, NMLD13, PHK14, RAGL11, RIJ+11, SJZ+15, VV+15a, VHS+19, YZG14b, YWZ14, ZWW10, Zim15]. translationally [MRO17, MK19]. translocation [BF19a, BGS+19, OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JSF19, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, MKK+19, NMLD13, PHK14, RAGL11, RIJ+11, SJZ+15, VV+15a, VHS+19, YZG14b, YWZ14, ZWW10, Zim15]. translationally [MRO17, MK19]. translocation [BF19a, BGS+19, OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JSF19, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, MKK+19, NMLD13, PHK14, RAGL11, RIJ+11, SJZ+15, VV+15a, VHS+19, YZG14b, YWZ14, ZWW10, Zim15]. translationally [MRO17, MK19]. translocation [BF19a, BGS+19, OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JSF19, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, MKK+19, NMLD13, PHK14, RAGL11, RIJ+11, SJZ+15, VV+15a, VHS+19, YZG14b, YWZ14, ZWW10, Zim15]. translationally [MRO17, MK19]. translocation [BF19a, BGS+19, OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JSF19, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, MKK+19, NMLD13, PHK14, RAGL11, RIJ+11, SJZ+15, VV+15a, VHS+19, YZG14b, YWZ14, ZWW10, Zim15].
BSD18, BB11a, CCR18, CVT+11, CAP17, CSSB11, DK19, DWL11, DBK17, DFF+15, DJS+18, DCHL12, DLZ15, ESD18, EWK+13, FF11, FRC18, FLM11, FZL+19, FL15, Gar12, GRS15, GFPSD17, GMO16, GZM11, GRL+11, GRL+12, GMBX+16, GTZ+18, HASR+12, HNS16, HNYH19, HLW+17, HDL+17, HHI17, Hof14, HBL12, HYUS11, HJKJ13, HZSS17, HHWL17, HLEM18, Hug14, HRRH+17, Ish10, IHJ+13, JLH+14, JMS13, KV13, Kan15, KSO+19, KERY+16, KT10, KLOS10, KGJZ19, KTNN10, KP11, LBGS16, LPK16, LRvdSM15, LZ12, LCH10, LCL+10, LMR14, LHE11, LTA+11, LBDP12, MS17, MZZ11, MJC14, MN15, MY17a. using [MHO18, MSS+13, MK19, MKM+17, MUJ15, MVKS10, MKB+13, MFR+17, MIOM13, MMJ10, MS18, NLP16, Nav18, NASH15, NHN16, OHPR18, OCW+15, PGdO+16, PC11, PG15, Pie14, PJ13, RB13a, RD18, RLDJ17, RDDS10, RHJ11, RvM19, RS13, RRK14, Ric16, REL17, REV+17, Rui11, RFHG10, REH13, SHMO11, SSO19, SzdB19, SFM14, SFD+17, SBV10, SA13, SW11, SEF+16, SHL19, SS19, SLK13, SB18, SY11, SRS14, SH19a, SZS16, STS15, TYZ+16, TYX+18, Tak14, TKNN10, Ts17, Th19, TJB12, UTM11, VKAM12, VECT12, V17, WKL12, WDN12, WLC12, WZ17, WXY+10, WDH13, XTY+14, XXY+17, XWW+11, YWJ+16, Yon16, YN15, YDX16, YFH+19, ZLD11, ZLT13, ZMX19, ZWS+10, ZP13, ZHI2, ZZZ+19, ZHXX11, dLC17, AIM+18, JCHT18, LHL+10]. utility [YHVM12].

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ARLP13, BZB+13, CJPTC18, DOM+11, DHF+11, DT19, EB18, HYD10,
IY18, KKA+18, KCPMG12, Kow11, KKH18, LBH+11, LLTC12, LBT12,
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SMF+18, VKC10, YZZ16, YD17]. virtual-bond-stretching
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voltage-dependent [SFBT17]. Volume
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Ano13y, Ano13y, Ano13z, Ano13z, Ano13-27, Ano13-28, Ano13-29,
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Ano13-92, Ano13-93, Ano13-94, Ano13-95, Ano13-96, Ano13-97, Ano13-98,
Ano13-99]. Volume
Ano18q, Ano18r, Ano18s, Ano19a, Ano19b, Ano19c, Ano19d, Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j, Ano19k, Ano19m, Ano19n, Ano19o, Ano19p, Ano19q, Ano19r, Ano19s, GY10, KRSC12, KTSW11, MK11, NASH15, NW17, Pop18, SZTSM10, Yan14, ZKE17. Volume [Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j, Ano19k, Ano19m, Ano19n, Ano19o, Ano19p, Ano19q, Ano19r, Ano19s, GY10, KRSC12, KTSW11, MK11, NASH15, NW17, Pop18, SZTSM10, Yan14, ZKE17].

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SLB12, TFO+11, YS13, ZYLL12, ZLLL12, ZLX+19, BSF18,
FZY+12, FL11, IJR16, KOP15b, LLOBO12, LHS12, LZL+15b, LCWW10,
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Yesselman:2012:MAT

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Yamada:2013:FPR


Yang:2013:FPS


Yu:2010:RPC


Yoshizawa:2013:NSC


Yosipof:2015:NNO


Yagi:2018:SMP

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Yang:2012:GAN


Yousfi:2010:REM


Yang:2012:MZE


Yu:2012:IDC


Yu:2012:AIM


Yanez:2017:FFG

Yan:2012:ESL


Yang:2013:RNI


Yang:2016:SNUa


Yang:2014:VSP


Yuan:2017:DSM


Yamabe:2014:MCR


Yuan:2015:MDD


Yuan:2018:MIW


Yang:2019:ITD


Yang:2013:DCS

REFERENCES

Yang:2011:IIZ


Yang:2016:SNUb


Yuan:2017:VWH


Zhao:2015:DMM


Zhao:2018:ABD


Zabojnikova:2016:IPS


Zhou:2015:LVS


Zou:2018:OLR


Zhao:2012:SNU


Zhou:2018:RPA


Zhu:2019:TSP


Zhang:2019:CBU


Zhu:2012:CEE


Zhang:2011:SSE


Zhang:2012:REFb


Zhang:2012:REFa

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[Zimmerman:2015:SET]

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Zhang:2014:ECM


Zhu:2010:PEF


Zoboki:2011:ELN


Zhang:2012:IRE


Zhong:2013:BST

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**Zerbetto:2014:LSF**


**Zarycz:2016:CSB**


**Zhu:2014:TPC**


**Zhang:2019:FTD**


**Zilberberg:2010:POD**


**Zapata-Rivera:2011:ESR**


Zhao:2011:CDL


Zhan:2017:ASE


Zhao:2013:FPC


Zahariev:2014:FAM


Zarate:2018:ERT


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Zhang:2013:MPI


Zhang:2011:ABD

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**Zhang:2011:IIR**


**Zhao:2011:HMM**


**Zhang:2019:GCH**

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Zhang:2010:ESO


Zhao:2014:IDB


Zhao:2014:DSE


Zhang:2015:TCS


Zhu:2012:PPT


Zhang:2010:III


Zhou:2012:CMF


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Zhang:2010:TSRb

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**Zhang:2012:RMC**


**Zhu:2011:CSE**


**Zhang:2016:CQD**