Title word cross-reference

\( (N-1) \) [ACD\textsuperscript{+}13a, ACD\textsuperscript{+}13b], \( (\sigma^3, \lambda^3) \) [TR12]. \( (\sigma^3, \lambda^5) \) [TR12]. +
[CXW14, GTK10, NMLD13]. 0 [UD12]. 1 [MG15, TS15b, YZLZ18]. 1 – \( n \)
[CYG\textsuperscript{+}15]. 10 [AC11b, TS15b]. 13 [WYGW12]. 15 [AC11b]. 17 [GZZ12]. 18
[LW16]. 2
[CWT\textsuperscript{+}12, GSS13, MSBF16, MH10, SJD14, WvRSM14, YDL\textsuperscript{+}10, YZLZ18].
20 [AC11b, LYL16, YVEI\textsuperscript{+}17]. 24 [TS15b]. 3
[AARP17, CM16, DVVP14, GMMH\textsuperscript{+}16, GSS13, GPK12, GBG\textsuperscript{+}19, HSW\textsuperscript{+}19,
LTT16, MG15, MA16, MYT\textsuperscript{+}14, MP19a, MSSP17, PSS14, Pop18, RVCFF13,
TS15b, VVMY18, YLL11, YZLZ18, dLvNC18b]. 4
[AFSW16, GWJJ12, ZTH\textsuperscript{+}15]. 4d [Hil13]. 4f [Hua16]. 4 \times 4 [LGKS17]. 4 \times 4
[SH14]. 5 [APY\textsuperscript{+}16, LZH16, YLL11]. 5\textsuperscript{+} [MKH15]. 6
[MCAY15, Rab12, TSZQ12]. 6\textsuperscript{2} [MKH15]. 6\textsuperscript{3} [MKH15]. 6\textsuperscript{4} [MKH15]. 8
[CSC\textsuperscript{+}18, TN12]. 8 \times 2 [LGKS17]. [2 + 2] [LXFC17]. [5 + 1] [YZL\textsuperscript{+}15]. [5 + 2]
[Ano10b, Ano12u]. 263fb [AR10]. 28 [HNWF12]. 2C9 [SLY+10]. 2D
[DAB16, DLC18b, YMY+19]. 2D-[YMY+19]. 2D- [YMY+19]. 2G12

3 [MWJ+11, DH17, HPSKI2, Spr10, YZGS14b]. 3- [LZL+16, YZLZ18]. 3-13
3-alternate [ZWS+10]. 3-d [YZ15b]. 3-dihydropyrido [YZ15b]. 3-Dipolar
[YN13]. 3-metal-carbon [ZYW+16]. 3-methyl-7-azaindole [YYT12].
3-squaraines [AMQ+14]. 3-thiophenic [NHF+10]. 3.0 [SvLK18]. 31
[ABB+13, CHR+12b, ICS+13]. 35 [SFCCK+15]. 36 [SMM15a]. 38
[HLS18]. 3c [KV14, LW16]. 3c/4e [LW16]. 3D [HSB+11, SA10, YMY+19].
3z [PTK11].

4 [YLZ+10, LTV10]. 4’- [YLZ+10]. 4-addition [KSO+19]. 4-amino-1
[ZZWT12]. 4-aminophthalimide [WHL+10]. 4-azaborinine [RS17a].
4-dihydro-1 [RS17a]. 4-hydroxyphenylpyruvate [DGH+11].
4-methoxybenzyl [YZLZ18]. 4-substituted [SKGB13]. 4-triazol-3-one
[MdOdQ18, MdOdQ18]. 4D-QSAR [MdOdQ18]. 4e [KV14, LW16]. 4Fe
[PN13]. 4S [PN13].

5 [SC18b, ZZWX11, cCVG+14, LL10c, Mor15, Pon10, SOvG12]. 5-b
[YLZ+10]. 5-biphosphate [CKG18]. 5-bridged [ZZWX11].
5-nitroiminotetrazolate-based [ZYL+12]. 5-phosphate [SY1].
5-triazine [WDLG12]. 5-triazines [YPC+10]. 5-triene [ABDGN12]. 53A6
[PVFL14, LG11]. 54A7 [LvG13c]. 56A6 [PLH16].

6 [WDLG12, ABM+15, TKN13]. 6-311G** [TKN13]. 6-31G** [TKN13].
6-bisphosphatase [RAR+11]. 6-fluoroquinolones [MPNS13]. 6-tetra
[WDLG12]. 6-trinitrotoluene [SH14]. 6-triphenyl [AS18]. 6.0
[GLW13a, GLW13b]. 60th [HIS17].

7 [ADF+10, MBR+15, UGK18]. 7-azaindole [YYT12]. 7-diphenylamin-9
[FWS+18]. 7-tetraene [ABDGN12].

8 [AAC+16]. 8-formyl-7-hydroxycoumarin [LZWH11].
8-naphthoquinone [HFWB19]. 8R [BG13].

9 [Sch10, Spr10, SOvG12, ZQ14]. 9-dimethylacridine [FWS+18]. 978
[ZQ14].
= [ATP18, ATIP18, ASS+17, AM19, CXS10, EPH+15, GPK+16, GNI18, JLH+14, JJAEB16, JJI16, LDJ+10, LLL+11, LJJ+11, Li14a, Li14b, LGW12, LLX+19, LZSM19, LCWW10, LWD13, MP19a, MCK17a, MCK17b, OKY18, PGS+15, PMG+16, Rab12, RDT14, SPS+12, Sak18, SIT18, SLIB12, TLdG+12, TFQ+11, TT18, TG12b, UT15, WWKS16, XhD15, YW12, YLT+19, YS13, YHCS11, ZYLL12, ZLLL12].

achieving [NNK+16]. Achim [Spr10]. acid
[BLG11, CYY+17, CC18b, CFC15, CM16, CB11d, FD14, FZL+15, Fell0,
FP17b, FCE15, GRL+11, GRL+12, HPT16a, HNN+17, HGY15, HCP15,
KSNT19, KLS10, KMLS10, LBC+12, LXL+11, LFMI2, LP11b, LPMI17,
MSLS10, MRO17, NHF+10, OXBIW16, PHDH13, PG18, SISK10, SZBM13,
SGY+18, SBW12, SV11, TKCN19, TL16, VMP17S, WC14, WG12, XN17,
ZSB+11, ZWP11, ZHIX11]. acid-arsenic [KSNT19]. acid-catalyzed
[CYY+17]. acid-phosphoric [KSNT19]. acid-water [TL16]. acid/base
[VMP17]. acidic [CYY+17]. acidities [ALK+15]. acidity [CRZ+18, CPK12].
acidity [AKL15]. acids [BSG+18, CCCLCGRO14, DKE+17, EHSPT16,
FCE15, GREA11, RSL16, SCF+19, SST+18, XLYZ10, ZKH10].
ACP [STM+15, SJ16]. across [AAC+16, GMPB12, MGS+16]. acrylate
[LZL+16]. act [LC10]. acting [BT18]. Actinide [SvLK18, RTS+13].
action [XLY12]. activated [CV12, FWS+18, KSR17]. Activation
[Niz13, AALCM11, DR11, DSM+11, FB12, LSL+19, MRR11, MBFG15,
PG18, TM18, TS15a, WC11, XLYZ10, YXZZ17]. activation-strain [FB12].
activator [BM12]. active [AIGP15, BHF+18, Cas13, DAP+18, DBP+12,
EB18, LVT10, NH19, PDG+16, SCSW13, SC18b, XTn18]. active-site
[DAP+18]. active-space [NH19, PDG+16, XTn18]. actives [EOO+16].
activities [AHK+19]. activity [BPC13, DKL+10, GAI13, GHL17, GFP17,
MJLV14a, RCM+13b, SLY+10, TD10, TBB+11, YB13, ZA10, ZD18].
acute [TTL+12]. acyclic [NMH19, ZKH10]. acyl [PS10]. adamantane
[EHSPT16]. adamantane-based [EHSPT16]. adapted
[FF11, SSSM15, TH13, YKH15]. Adaptive
[ISK14, KEMP17, LZZ+17, AOW11, BGR13, DSK17, FHMB15, HDM+15,
LL19, MJC14, MBFP15, MJG+15, OZI4, PN13, SNS13, WTD+19, WMW+10].
Adaptive-numerical-bias [KEMP17]. adaptively [ER18, SR18].
adcluster [IN13]. Adding [XHLH16, PFAS+19, Zha12b]. addition
[FWB14, KSO+19, KS13b, NDG14]. Additive
[XVA+16, DPNM11, HM13, TSR+16, VPA+10, VMP17]. additivity
[VRKT19, ZRL+15]. address [LG14]. Addressing [MMH19, cCVG+14].
adduct [KK19]. adducts [LC10, LS11b, ZRCC11]. adenine
[BZH14, LLT12]. adenosine [SRA17, WZQW10]. adhesion [Won18].
adhesive [HTY19]. adiabatic [MT19b, UD12]. adjacency [GZH10].
adjusted [HH15, KHL15]. Adjustment [BLZ+13]. ADMA [MA17].
AdNDP [KDS17]. adrenergic [CV12, LLHM16, VKC10]. adsorbate
[GBS+17]. adsorbate-induced [GBS+17]. adsorbed
[MF10, PXXW10, SLL13, SIG+15, TH1+19]. adsorbents [HV16].
adsorbing [KGZJ9]. Adsorption [CCJ+11, FVP14, HB15, KD10, LH14b,
PH12, AS15a, BS16b, CMM18, CR14, cCVG+14, Hei10, LL13a, LPK16,
LPLS16, LZ14, LT14, LCM+14, NPP13, PC12, PLZ17, RHNN10, SH14,
SDS+16, SKTT11, SYZ+17, VS14, WSW15, WYGW12, YDR13].
Adsorption-induced [HB15]. Advanced [WBN+13, Yan16, DJs+18].
affect [SV15, UNT16]. affected [MCF+18, OHNK11]. affecting [GMSV14].
affects [CLK11]. affinities
[CMD13, CTP13, GRS15, MGWR12, NHN16, NFG+13, PBLdS12, RJWW12, RMGB11, VCL18, VKC10, WNP+16, WLLL18, SDIP18]. affinity
[CG15, CZAFL7, DLZ15, MUGNVJ+18, MCK17a, SSP+13, VL17a, ZJZM13, ZYvIZ14]. After [WZK+13]. Ag [LLX+19, Rab12, ASl5a, BBG+18a, IN13, LLTC12, MCF10, PGS+15, SLL113, TNI+19a, THI+19, YXZZ17]. Ag-nanocluster [AS15a]. against [Gil11, MPNS13]. Age [Yan16]. agents [PSdPE+10]. Aggregate [NNT+19]. aggregated [BSL+16]. aggregation
[RCR+13a, RML+15, WDP+12, ZSTRS+18, PK19]. aggregators [RLL+10]. Agonist [HK18]. agonists [CV12]. AgX [YS13]. AHAS [SJD14]. aimed [KS12]. Al
[LCWW10, Pon10, UT15, YR13, CC18c, GWJJ12, KKR+13, SH14]. Al-hydroxylated [SH14]. Ala [SZBM13]. alanine
[I013b, LL19, MAMF19, MVKS10, SEM12]. AIB [MCAY15]. albumin [JAH5+19]. alchemical
[BBI11b, BBI1c, BG12, GMSdG15, GRS15, HLW+17, KB11a]. alcohol [MS13, ZSZ+14]. alcohol-based [MS13]. alcohols [VVLG17]. aldehyde [ZZWT12]. Alder
[CC18a, FB12, FB14a, GNDA+12, LZH16, ORZ11, ST13, dSVdM+16]. Alder-ene [FB12]. Alderase [BJSI12]. aldonol [HJLV16]. aldosterone [RVP+11]. algebraic
[GJMPAM+14, WWD15, YD17]. algebraic-diagrammatic [YD17]. Algorithm
[WM12, AMGB10, AM10, AYYO17, BW11a, BYE+16, BDD13, CM13a, CDBM11, CGA19, CTV+11, CM13b, CB11b, DS15, DJ13, DLSA14, DZA11, EVR18, FRLN10, FGFI1, GPE13, GBFD12, HTS15, HEMCZE+14, HQC16, HKR+14, Hug14, Ish10, IJJ+13, JCPC11, KK17a, KNHN16, KN17, KD18, KDT+12, LZX16, LLI+13, LZLMP16, LSS+17, LLIJ12, LTA+11, LMA15, MEH18, NYN17, NC12, NG10, dRL11, PS17, RPMAM15, RAs17, RSL16, SSO19, SRSLO15, SYH12, SSMW09, SCSW13, SA11, UCRL18, WMW+10, XHLH16, YVEI+17, ZSS+13, vLBBR12]. algorithm-artificial [WMW+10]. Algorithmic [LPS12]. Algorithms [BV14, KGHC15, AGR11a, AC12, CD13, Fom11, GBSE11, KJM+17, Lehi15, LLZ12, MS16, MO15, NC14, NOKJ16, RFN15, TRA+16, ZVY+15, dACP12, vLBBR12]. aligned [KC14]. alignment


amination [YZ17]. amine [AK10, BMB13]. amines [MRC+18]. amino [BG+18b, CCCLCG14, CFC15, CB11d, DKE+17, FZL+15, FP17b, GRL+11, GRL+12, HCP15, KLS10, KMLS10, LXL+11, LP11b, MRO17, PHDH13, RSL16, SISK10, SZBM13, SST+18, WC14, ZZWT12, ZKH+10, ZHIX11]. amino-acid [KLS10, KMLS10]. aminoacid [MC10].


analyses [BSF18, KASH14, KP11, PZBA13, SKGB13, VVJ15, XWW+11]. Analysis [CDM+15, HAI+16, JCGM18, LL19, MOS12, SvLK18, XFG+16, AKMT11, AST+16, ASL+11, ARRC15, AS18, Aon15-58, AM19, BK15, BH14, BSPP+13, BBG+18b, CLFR018, CMM18, CAF+13, CEBO15, CCC+11, CAT+13, CH14, DMJ17, DDP+18, DHF+11, DJD12, DBK17, DJS+18, DCS15, DN19, ESD18, EHSPT16, EB18, Fer17, FB12, FHW+11, FHK+12, GFP+10, GLW13a, GLW13b, GNDA+12, GCP+13, Han11, HSB+19, HCD+10, HPSKL2, HHT+13a, HHT+13b, HGW18, HDHL15a, HDHL15b, HDHL15c, HHWLL17, 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, MJC14, MT19b, MeI0, MADWB11, MCLD10, MGS+16, MCK17b, NK19, NH19, NIIT15, NS17, OXBW16, OC14, PTK11, PSP15, PRYI+17, PTB+15, PPUBGD10].

analysis
Analytic [Box18, MDTD13, NF18, SZX13a, SZX13b, TSH+19, WNP16, Wei12a, Wei12b, WDKT19, XFG+15, YK13, YNH+17, Yes12, Yes15, ZCS+15, ZBB16, ZH12, ZZX19, ZWX18, vSGP10, JCHT18, SZL19, Spr18, ZSB11] .

Analytical [CCR18, CCB15, HNWF07, HNWF12, HH17, LBGS16, SF17, WOH18, CHJ+13, FBY+17, HH16a, KN17, KT5W11, MK13a, Pon11, Pop18, ZWF15].

analytics [JZL17].

analyze [LP11c, OVPK15, QLQ11, RLG14, YKO+11, dVAG16].

analyzer [JJW+14, LC12, PVZ13].

Analyzing [BD11, MRB14, BCP10, HPT17, LZS17, PHT17, SWA13, WES13].

anapole [ZPP+16].

anatase [HRL11].

and/or [KB10, Pog10].

androstenedione [VCM15].

angle [CKP10, GBFD12, XML+15].

angle-dependent [CKP10].

angular [BBG+18b, ENKK+17].

anharmonic [Kow11, SSWX14].

anhydrase [SSP+13].

anhydrides [RB12].

aniline [PLP16].

Anion [TT18, CG15, KSNT19, LC10, uLhY11, LCC18, SC18a, SDF12].

anionic [AM19, GZZ12, GH13, HPL13, JCP14, QZ10b, ZYR+15].

anionic-water [JCL14].

anions [PVS12, RDT14, RJS17, ZYW+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 [RHJ11, SHMO11, SHL+11, ZC14, LMZ11a].

annihilation [BL12].

annulated [RS17a].

anode [GNI18, YZLZ19].

anomerization [SM17].

anomers [HH11].

ansatz [Bou14, WGA18].

answer [SJWE10, Tan19].

ant [ZsA10].

antagonists [LLL+10].

anthrax [JA+17].

Anti [WFZ+18, ZsA10].

Anti-Electrostatic [WFZ+18].

anti-HIV-1 [ZsA10].

antiaromatic [TDKT10].

antibiotics [PG15].

antibody [UNT16].

anticancer [SZ+18].

antiferrromagnetic [ZB18].

Antiferromagnetically [SZL19].

antigen [JA+17].

antimicrobials [PPUG10].

antioxidant [GAI3, ZDW18].

antiparasitic [PPUG10].

antisense [ICS+12, ICS+13].

antityrpanosomal [PSdPE+10].

antitubercular [TD10].

AO [YOPB16].

AOFORCE [vW11].

APBS [UH+11].

API [LAS+14, ZW18].

AppA [XBS19].

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, MH10, OLI13, PAK15, RVP+11, Smp17a, SRS14, SC17, SDL14, SMM+18, VKTJ15, WH11, ZsA10, vSGP10, CSAdOM17, CJP1CT18, DP1M14, Eik16, GLL16, GFG11, GCW16, IUK+11, KT19, KFY+13, KS18, KS11, LLHM16, LP11a, LLL+10, LLLC11, Lvg13c, MDTD13, MDOD18, PHC13, RZG+13, ZC14].
As-Rigid-As-Possible [NJR18]. AsCl [MLCD11]. ascorbate [HHDC16].
ASED [BRP+12]. ASED-MO [BRP+12]. Asp [LY10]. asparaginyl [LBS10].
[ABB+12, ABB+13, ECZWD17, NC13, NC14, OPR16, Tac19, VKNT16].
assembled [KC13b]. assemblies [AKK+16]. assembling [AFSW16, CD11].
assemblings [CBTZ16]. assembly [AGR11b, Hei10, JM11, KLN16, uLhY11, Mau14, OAN15b, TBJ18].
assessed [SJ16]. Assessing [HWLW11, KYB13, KSR+16, OCLM14, SNDK16, VL17a, FNSF+11].
Assessment [ARRC15, FB10, GKH12, HDK+12, HJ10, KB10, KB13, LSH+11, OOT15, SB14, UCFR16, WL10, WYT17, YB16, Yu12b, ZZZ+12, AR15, BG13, ED15, FCE15, FPRS14, FLM11, GAI13, ITIN15, LTT16, LZLC13, MS13, MFR+17, SZX13a, SZX13b, Tsi14, ZTH+15, HCB11, Sch12, YVEI+17]. assigning [LFB14]. assignment [Ben17, KKH19, MPBJ11]. Assignments [TT18].
assist [TS10a]. Assisted [DBGO+17, LL13b, SSGS15]. associated [WNM17, ZZ10, dLvNC18a]. association [DSF17, JA10, MBR+15, NC14, OCW+15, PD12].
associative [Ano10a, JLS18, SN10]. asymmetric [DLSA14, HAL14, KSO+19, NDG14, QLYL10, WCDM11].
asymptotic [KIOY19]. Asynchronous [XFG+16, XFG+15]. AT-rich [YZWC11]. Aten [You10]. atmospheric [BCNH+11]. atom [ATP18, BS10b, CVT+11, CS14, DPNM11, DM15, FSC+14, GBVA11, HRK+10, HM13, JYC+16, JGS+17, Jor17, KV14, KT18, LC10, LZZ14, LKZM18, MZZ11, Niz13, OCW+15, ST11, SM14b, SYH12, Tsi17, VIT+15, VHA+10, VKAM12, VI17, VDVR14, YPKB12, YHCS11, ZFS18, dLC17, dVZ17, YMP14].
atom-typing [YPKB12]. Atomic [BMFG16, EPD+10, KGM12, AYYO17, BLDK+13, BB11a, CCR18, CP15, EKH14, Elk16, EP12, EV14, HS12, HH18, JMLL13, JXS15, KHLM19, KOP+14, KR12, LRVM18, Lar11, LZGS11, MK13a, MPA10, MPA12, Mat10, MPBJ11, NPG17, NOKJ16, OBW12, OV14, Pol13, RB13a, SS16b, SE14, SMP17b, TSH+19, VSA11, WWCL15, YOMT14, dLC18a, dLvNC18b, VV19].
Atomic-resolution [BMFG16, NPG17]. Atomicistic [BH13, CHKR10, MTS+19, MBA14, SE14, BLKP12, CZNA11, DDP16, HDPM14, LZ12, MSC+10, MMZW14, RO14b, RSG+10, ZST14].
atomization [KSM17]. Atoms [JCHT18, ARAG17, ARLP13, BSF18, BSPAN+13, CGA19, DC13, EV14, GAMAC+14, HSJ18, HSB+11, HGCCGR+16, IN13, Jab18a, KHE+19, LHSH12, MP17a, Mit13, MyvBD18, PNE18, Pop18, Pyy13, SFCCK+14, SFCCK+15, STS15, TY10, VGV+11, VyB15, VyB16, WZH+18, WYZ14, YKH15, ZYW+16]. atoms-in-molecules [BSF18, HSB+11, YKH15]. ATP [BMFG16, SYH12, YHH+13].
ATP-binding [YHH+13]. ATP-Mg [BMFG16]. ATPase [II10]. atrazine [BHB+17]. attachment [HBL12, SSS+18, THP+15]. attack [MLY+13].
DVVP14, DH14, Dil15, DJX⁺11b, DJX⁺11a, DFF⁺15, DPB⁺12, DXL⁺10, DCs15, DDM⁺15, EFAC13, EHSPT16, EV14, EBK13, EP15, EBPK17a, EB18, FCL⁺10, FCQGM12, FCPJM14, FHZA⁺18, FMG12, Fra15, Fra16, GLZ16, GHL17, Gar12, GJMPAM⁺14, GJK⁺19, GBVA11, GC18, GVP⁺10, GN18, GSS13, GBSE11, GZ14, GK15b, HKRS11, HS11, HLS12, HH11, HTS15, HW19, HZY⁺10, HSW⁺19, HPL⁺18, HKR12, HB14, HEMCZE⁺14, HSB⁺11, HYUS11, HM13, HIWD15, ISN13, ISM18, JJW⁺14, JLCA17, KS18, KGH15c, KZZ⁺16, KLZ⁺18, KNE11a, KC14, KP11, KKHS19, LFB14, LX11, LM18a, LDB⁺17, LMZ11a, LMZ⁺11b, LWL⁺11, LLZA12, LSH⁺11].

based [LZS⁺17, LZSM19, LTA⁺11, LGKS17, MDTD16, MZZ11, MMM⁺16, MSY19, MC10, MA16, MDQ18, MGCC19, MPNS13, MMZW14, MAP18, MFR⁺17, MO15, MNNK10b, NC12, NC13, NC14, NMH19, NJX⁺10, NG10, OVPK15, OZLSBH12, PRP15, PLZ17, PSC11, PBBP11, PN13, PKC11, PPJ14, PLH16, PBE16, PUBG10, RLDJ17, RZG⁺13, RMRBH⁺19, RVP⁺11, SM14b, SFG⁺17, SLR⁺12, SLX⁺15, SGR⁺18, SFDE16, SLC⁺17, TYZ⁺16, Tak14, TTB⁺10, TS14, VGV⁺11, VVJ15, VC10, VSA11, Vor10, WXL⁺12, WLLH18, WCDM11, Wei12b, WL14, WS13, WDH13, WZWW18, XCLZ19, YJN⁺11, YZ16, YWJ⁺16, YZ16, YZL19, YDL⁺10, YJ11, YN15, YS13, YS15, YS10, YZZ⁺17, ZSLL17, Zha12b, Zha12a, ZY14, ZW18, ZM10, ZYL⁺12, ZT14, dCLFGL13, dSVdM⁺16, dVZ17, FAS⁺18, NKJ16, WTD⁺19, ZDW18, dLVNC18a, dLVNC18b].

based-on [CDS16].

bases [CWZB10, KASH14, LRVM18, MSLS10, SC18b, SBW12, WGA18, ZLL⁺10, Zha12a, ZBMZH15].

Basic [CMvG10, WLF19].

basin [JLH⁺14, RDRC16].

basin-hopping [JLH⁺14].

basins [SBN13a, dLC18a, SBN13b].

Basis [BLF14, BRLS08, BRLS12, PH14, SN16b, TK13, ACD⁺13a, ACD⁺13b, BLFZ13, BLL13, BLBG⁺13, BS10a, BLG10, CC11, DBM⁺15, DLZ15, Fer13a, HSN14, Hili3, HBL12, KKi7a, KT19, KN12⁺15, LDB⁺17, LBH⁺11, LCW12, Lehi5, LYC⁺13, LZ18, Mit13, OAN15a, PML⁺12, PGD⁺16, POB13, Pla11, PD11, RLD12, SWM10, SG10a, Sea10, SNKS10, SM18, Sun15, SG13, TH13, WX12, ZPP⁺16, ZLT13].

Batch [WHJH13, TJBJ12], bath [CSEM16⁺15, MO15, Vor12, WAM17].

BaTiO [BE12, EB12, EBK13].

batteries [GNI18, YZLZ19].

battery [SM19, QCR12, WvRSM14].

Bay-type [WvRSM14].

Bayesian [Fer17, GZ14, SGKP19, VZ14].

BayesWHAM [Fer17].

BD BOX [DZT11].

Be [GNI18, LDJ⁺10, LLX⁺19, EPH⁺15, IMSR18, KV15b, LZW⁺11, NDC14, SMGB11, TH13, TCPPC14, Zha12b, BWW10a, CC18c, CCM15, CM16, ZLY⁺16].

Becke [FPV13].

become [Tan19].

BeH [ZL⁺16, ZLY⁺16].

behavior [AVHB18, BVY⁺12, CME11, CSAdOM17, FCD10, FTR15, KRTB10, LZY⁺12a, PD11, TLDG⁺12].

belief [FPSD17].

Benchmark [CXD⁺19, WSZW15, AF14, ANH⁺11, CSXZ17, cCVG⁺14, DGSVGM19, GA114, KG15, NH19, RS13, ZWGO16, IKn13].

Benchmarking [XYW⁺14].

Benchmarking [Ben17, GA⁺17, Hug12, LCM⁺14, GP11b, HRJ⁺14, HRJ⁺15, HZ13, IY18, JRSHP14, KSM17, RSG14].

benchmarks [GPD⁺16].

benchmarks [HLEM18, XKW18, ZDK12].

bending
binding [TS15a, UNT16, VVG13, Vor10, VM11, VHS+19, WS10, WNP+16, WLLH18, WL14, XHLH16, YZ15a, YZZ16, YJXZ13, YHH+13, ZZ14, ZJZM13, ZYvIZ14, ZLX+13, dRBO13]. binding-based [MAP18].

binding-site [ISP+10]. binds [XHLH16]. BINOL [HPT16a].

BINOL-phosphoric [HPT16a]. Binor [WJX10]. Binor-S [WJX10].


BioLayer [JAH17]. biological [BHB12, Ben17, CLK11, DLL+10, DMN15, GREAI11, GFPSSD17, GLM+17, JS17b, LPLA13, Mat14, MG11, SCF+19, VHA+10, WCJ+14, SDP18].

biologically [BZH14, Mat10]. biomimetic [ZRCC12]. biomolecular [KMS+19, LZTV10]. biophysical [FN12, Mat14, RFP+13].


bipyrimidyl [ZLZ14]. Biradicals [SZL19]. birthday [HIS17]. Bis [WWKS16, KGR+16, KTK17, YMY+19, RHPWS13]. Bis- [RHPWS13].


blending [KM13]. Blind [Vor10]. Block [BGR13, Car14, CAT+13, EWK+13, MCK17b, TDKT10]. Block-adaptive [BGR13]. blockade [AB10]. blocked [KLS10, KML10]. blockers [CV12].


Boltzmann [ALRM18, BCCO10, BD12, CLA16, FBY+17, FMB15, FCE15, Fra15, Fra16, HWWL11, KB11e, NWW17, SK15a, WL10, WLQ19, XY17, YOM14, YLS19]. Bond [BVC13, Jab18a, NKD18, Pon11, SK13, WM12, ASL+11, AF516, BK17a, CFM+19, CPR+12, CR19, CVT+11, CD11, CKL+11, CP10, DR11, DBG11, DL19, EPF+15, FCPJ14, GREAI11, GCCM15, GLW13a, GLW13b, GCW16, GC+11, HS14a, HAI+16, HEM+17, JSW10, KTT16, KV14, KSNT19, KKA+18, KLS10, KML10, KSC16, LCPS13, LDJ+10, LLL+11, LZJ+11, LZY12b, LGKS17, MPSG11, MLGB16, MS11, MVBD18, NNF+10, Niz13, PKK17, QZM11, RHRCH16, RL11, RS17b, Rob13, RRK16, SZ17, SP13, SFA17].
SSWX14, SB18, SSMW09, SCSW13, TM16, Tan19, TD11, VECT12, Wei12a, Wei12b, XP13, YK13, ZWLX11, ZLT13, ZZW19, ZWF15, vLBBR12].

bond-order [ZW15]. bond-valence [HAI+16]. bonded [BLFZ13, BSD18, BLDK+13, DKT13, JCP14, LJW11a, LHHW14, LZSM19, PAT+10, SSGS15, UT14, UT15, WHX+10, ZZL+12, ZDX11, ZBMZH15].

Bonding [BP13+13, GRD+16, BD+13, KGR+16, ZLZ14, ZLY+16, ZB18, ZZWX11].

Bonds [WFZ+18, BT18, CXD+19, DGB+13, ED15, FPRS14, Gra18, HH15, Jab14, JJJ16, LHZ+11, LZL+15b, LZY12b, LDG+15, OOK11, Rob13, SM16a, SK13, SJ16, YLT+19, YLL11, YKH15, YJ17, ZLY+16, Jab18b, YLZ+19].

BonnMag [BBG+18]. Book [Sch10, Spr10]. boost [KV15a]. BOP [SH19].

borafluorenes [ZQ14]. borane [BEPM14, Kop15b, LC10]. borates [GWJJ12]. borides [ZWMW10].

born [AB16b, BLZ+13, DSF17, FCE15, HWLW11, KCPMG12, LL10a, LCH10, MT19b, PS13, RSB+13, SZTSM10, SSBW14, VMPS17, WWKS11].

boron [BEPM14, Gra18, GAMAC+14, LT14, Olt16, PGC12, VS14]. boron-doped [VS14]. boron-nitride [LT14]. boryl [LC10].

BOSS [VKTRJ15]. BOSS-Gaussian [VKTRJ15]. Bosutinib [GMASBF16]. both [AST+16, FNSF+11, LX11, TH13, WZ19]. bottleneck [SRR16].

bound [FLM11, GPK+16, LFM12, MAK+14, PMG+16, PZA15, XWSW13].

boundary [KB14a, Lun12, MTvG12, NO16, PL14, PS13, SSP19, Sie15, VECT12, YAO18].


Boys [WO15]. bptz [CWT+12]. bpy [LWXC16].

Br [ATP18, ASS+17, EPH+15, GPK+16, LDJ+10, LLL+11, LZJ+11, PMG+16, YS13, ZLL12, LZL+15b, MKH15, MPSBC19, XhD15, ZWY+10b]. Branch [Ish10]. branching [BEL+11, OZLSBH12, STM17]. BrBr [LGW12].


Bridging [YLL11, dCDP15, LLL+11, MIP+15, BPC13]. Brillouin [QS19].

Bringing [RR11]. broad [MP19b, TZ12]. broken [KKW18].

broken-Symmetry [KKW18]. bromide [MG15]. bromination [SGS+16].

Bromine [LWL+16]. BROMOC [DMN15]. Bromosuccinimide [QQY+18].

C [LdSRR16, LTR18, LAHS16, LLD17, LCWW10, LWD13, MLQ+12, MCK17a, MCK17b, NKD18, PMG+16, RLA+11, Sak18, SKMS13, STS+10, SBW12, Tak11, UT15, WCY+11, WKK15, YZZ+17, ZYG+14, ZLY+16, BS16a, VAMS14, AM19, Ben17, BWK10a, BS16b, BH13, CG12, ED15, FL15, GWT+17, GMS14, GZZ12, HJ13, HVS16, IMK+16, JLS+10, KV14, KP10, LFB14, LC17, LDH+14, MSV16, MH11, MSPC19, Niz13, OPR16, PTK11, Pie14, PZB13, RWR+13, SND16, TFQ+10, TFQ+11, TS15a, TKN19, VAR12, VED10, WK10a, W10, WWT19, WL14, WTH+16, Yes12, Yes15, YDZ15, ZZZ+19, ZZL19]. C-terminal [IMK+16].


EFAC13, EK17, EWK^+13, EP12, EB12, EBAK13, EB18, FAA15, FRC18, FA18, FE14, GRARO^+14, GA18, GMO16, HASR^+12, HYL^+11, HS14a, HB14, HSH15, Heli13, HG10, HG13, HBL12, HYUS11, HGW18, Ibr17, IMSR18, 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, LYG13b, LCK^+18, LCM^+14, Lun12, MK17, MK19, MUGNVJ^+18, MLN^+18, MCLD10, MEH18, MCK17a, MCK17b, NWW17, NZM18, NLL19, NCT18, NN18, OHNK11, OLA15, OOT15, OZLSBH12, PBLdS12, PTK11].

calculations [PHK14, POB13, PBBP11, PDG^+16, PN13, PGW^+17, RAR^+11, RLZ^+18, RHT^+15, RLD12, RR11, REV^+17, RH10, RK15, SH15, SRSLO15, SP13, SPHF^+18, SS16b, SCW11, SWPR11, SRS14, SMP17b, SDMS13, SHB17, SIK11, SPZP18b, SPZP19, TLdG^+12, TNY18, TS10a, TN19b, UHH, VLB^+10, VKAM12, VKNT15, WK12, WHK^+12, WTH^+16, WGA18, WXY^+14, WYJ^+16, YD17, YN15, ZRCC11, ZLT13, ZLZ14, ZWMW10, ZH12, MSPC19, NQB19].

calculator [dCLFGL13].

calibrate [VVLG17].

Calibration [CBP14, DDM^+15].

calix [GMASBF16, PRRT^+10, YCGA10, ZWY^+10a, ZWS^+10, GMASBF16].

Can [ZPF14].

CAMERRA [JLS18].

Can [ASMS10, IMSR18, KV15b, LZW^+11, NH19, PLAG11, SHL^+13, SPZP18a, CIKT13, LCB10, TCPPC14, Zha12b].

CANADA [Fel10].

cancer [NS10, WC11].

Canepa [LHMM11].

cannabinoid [ILKR11].

Canonical [CPN^+17, RHNN10, BW11a, HRK^+10, KCK^+17, PHH^+12].

Canerakis [UCRL18].

CaO [BL12].

CAP/SAC [EFS16].

CAP/SAC-CI [EFS16].
capabilities [AAC^+16].
capability [LC10].
capacity [KOP^+14, PGC12, WK10a, WKLC12].
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, LXX^+10, TCPPC14, WS11, WS12, dSdlBNB17].
carbenes [BAD^+19, BSDP16, KYKR15, RF15].
carbocation [ONTTL16].
carbocations [OPR16].
carbonyl [BAD^+19].
Carbohydrate [ZYvIZ14, NMF^+14].
Carbohydrate-binding [ZYvIZ14].
carbohydrates [CP15, HH11, JSD^+11, PLH16].
Carbon [SC17, AS15a, AAMR18, AS15a, BPE16, CME11, DI11, Den12, DC13, Fom13, FTR15, GMSM15, GPK^+16, GBS^+17, GZ12, JW01, KGHK12, KV14, KPH^+19, KHE^+19, KGJ12, LPLS16, LL10c, LT14, LK16b, MSY19, OCW^+15, RHNN10, RRK16, Sie18, TSR^+16, VS14, WYL^+15, WDZN16, YNZ13, YZZ^+17, ZY^+16, ZYL^+16, ZWF15, OSI^+19].
carbon-beryllium [CME11].
carbon-carbon [KGJ19].
carbon-germanium [GSM1M15].
carbonate [ZSWL12].
Carbondioxide [Sea10].
carbonic [SSP^+13].
carbons [MBK^+13, RVB^+12].
carbonyl
carbonylation [MRC+18].
carbonyls [SSX+14].
carboranes [HJ13].
carboxybetaine [DQ16].
carboxylates [AARP17, RVM19].
carboxylation [CKG18, DGSVGVM19].
carboxylic [LPMT17, RB12]. card [SR11].
Carlo
[LHMM11, NQB19, Aou16, BFH++13, CLK11, CG12, CTP13, CAP17, DMMN15, FFA14, GP12, GPM17, HFSO12, HMM10, HYUS11, HQC16, HHBY10, IHJ++13, LPK16, LMZ11a, LZ12, MS16, MBRC16, MOS12, NDW15, OPFR17, PSS14, PS13, Pon10, PIH++12, RHNN10, RdA12, SCOJ13, SAGC16, SMRM++17, SSSP19, SE14, UU12, ZLM++15, ZW17].
Carlo/Brownian [DMN15].
Carlo/molecular [RdA12].
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].
cases [GREA11].
CASPT2 [LGZ15, SGWA17, VFRAR16, WGA18].
Cassandra [SMRM++17].
CASSCF [KKL++13, LWGZ15, NH19, SGWA17].
CASSCF/CASPT2 [LGZ15].
CASSCF/MC [KKL++13].
CASSCF/MC-XQDPT2 [KKL++13].
CAST [GBW++14].
catalysis [Can10, Can11, EvRC++18, KK19, LHMM11, MG14, RNS19].
catalyst [BEM14, DK19, DSHLM18, LLCL17, RLZ++18, WWTL19, YZ15b, ZSWL12, dSDdAR10].
catalysts [AHK++19, BEPM14, JJAB16, NJX++10, WJX++10].
Catalytic [YMY++19, AHK++19, GHL17, GA19, KV15b, ONTTL16, SJ14, SLY++10, SOYC12, TM18, UKS11, WZQW10, dSDdAR10].
catalyzed [AS11, BF19, CYY++17, CCJC10, CPLLI1, HPT16a, HDB15, HJLV16, KSO++19, KB13, KT12, MRC++18, MG15, MTS++19, QLYL10, TLA10, Tsi17, VCM15, WCW11, WWTL19, WXY14, XLYZ10, XXZ17, YZ17, YZLZ18, dSDdAR10, dSDLBNB17, dCDP15].
catastrophe [ABDG12, GND+12].
catechol [PBLdS12].
catechol-O-methyltransferase [PBLdS12].
Catenanes [LAHS16].
cathepsin [ETLS17].
cathode [SMiN++19].
cation [CCCLCGRO14, CGPP11, DLMLH12, DDM++15, RMGB11, SSGS15, ZYL++12].
Cationic [HJ13, CI18a, WJX++10].
cations [CC18b, KGR++16, LCL++10, LDsRR16, LTR18, PVS12, SD++17, Tac17, THP++15, ZWY++10a, ZWS+10].
cations/nucleobases [CC18b].
causes [GDV17].
cavatand [CC18a].
cavities [HRB++17, ZSB++16].
cavities/vacancies [HRB++17].
cavity [KD18, ZWS++10].
CAVS [SDZ17].
CB [BTMS12, CC18a, ILKRN11].
CBS [KG15].
CBS-QB [KG15].
CC [Gil11, LLTC12].
CC2 [SGWA17].
CC3 [LZ14].
ccCA [RJWV12].
CCSD [BBI++11, MSPC19, CGOA17, Gil11, KK17a, KKL++13, MVKS10, OPR16, PC14, RS13, SRR16, SB14, XKW18, YJ17].
Cd [SLIB12].
CDocker [GLB16].
C == [CROB16].
CsS [NS18].
Ce [Ibr17, YOPB16].
CeF
[KKA'18]. cefotaxime [MFM+12]. cell
[ACS12, CGBK13, Elk16, Fom11, Gon12, JMS14, SRL+15, VÂA14, dACP12].
Cells [FPV13, ACS12, DZA11, DGL+13, JYS+12, LZL+15a, SV11, SLC+17, TZ12, YJN+11]. cellular [VBD11].
Cellulose-Builder [GS12]. cementite [VED10]. cementite-type [VED10].
cementitious [TZ11]. CENCALC [SDMS13]. cenus [PPUBGD10].
center [CXD+19, IIF+10, LRER13, YLL11, Yu12b]. centered [FA18, VI17].
centers [Gav12, GA19, WC14]. centered [FA18, VI17].
centers [Gav12, GA19, WC14]. central [DGL+13, Yu12a]. centrality [RNVP13].
centre [SC18a]. centric [LABSG17].
cementite [VED10]. cementite-type [VED10].
cementitious [TZ11]. CENCALC [SDMS13].
census [PPUBGD10].
center [CXD+19, IIF+10, LRER13, YLL11, Yu12b]. centered [FA18, VI17].
centers [Gav12, GA19, WC14]. central [DGL+13, Yu12a]. centrality [RNVP13].
centre [SC18a].
centered [FA18, VI17].
centers [Gav12, GA19, WC14]. central [DGL+13, Yu12a].
centrality [RNVP13].

Cellulose-Builder [GS12]. cementite [VED10]. cementite-type [VED10].
cementitious [TZ11]. CENCALC [SDMS13]. census [PPUBGD10].
center [CXD+19, IIF+10, LRER13, YLL11, Yu12b]. centered [FA18, VI17].
centers [Gav12, GA19, WC14]. central [DGL+13, Yu12a]. centrality [RNVP13].
centre [SC18a]. centric [LABSG17].
cementite [VED10]. cementite-type [VED10].
cementitious [TZ11]. CENCALC [SDMS13]. census [PPUBGD10].
center [CXD+19, IIF+10, LRER13, YLL11, Yu12b]. centered [FA18, VI17].
centers [Gav12, GA19, WC14]. central [DGL+13, Yu12a].
centrality [RNVP13].
centre [SC18a]. centric [LABSG17].
cementite [VED10]. cementite-type [VED10].
cementitious [TZ11]. CENCALC [SDMS13].
census [PPUBGD10].
center [CXD+19, IIF+10, LRER13, YLL11, Yu12b]. centered [FA18, VI17].
centers [Gav12, GA19, WC14]. central [DGL+13, Yu12a].
centrality [RNVP13].
centre [SC18a].
centered [FA18, VI17].
centers [Gav12, GA19, WC14]. central [DGL+13, Yu12a].
centrality [RNVP13].

[CFM+19]. CH/ [OOK11]. chaff [NMF+14]. Chain
[vRWGS17, BFH+13, CHKR10, DMD+18, HAL14, KV14, KLS10, KMLS10, LPS+13, LZGSI1, LP11b, LvGI3a, LZMP16, OZ14, PD12, PS10, QZM11, SA13, SISK10, SZBM13, TSN16, DKV18].
chains [AFSW16, FP17a, JSW10, LZZ14, NPP13, Pla11, PLH16, TLDG+12, TS15b].
chalcogen [CFM+19, DDP+18]. chalcogenides [SPS+12]. chalcone [CPLL11, YZ17].

change [EMD17]. changes [GDV17, GBS+17, HB15, LK13, MJLV14b, MO17, PdSC18, RO14b, YZGS14b].
Changing [XVN17, LLvG10]. channel
[HYYZ+13, PVL+13, SFBT17, SY16b, TCX+13]. channels
[KC13a, LL10c, NSK18, OKIS17]. character
[Ali18, BMB13, Cas14, Ibr17, LCK+18, RIJ+11, VSH19, YSSB12].
characteristics [DPSL16, Gav12, LT14, Mat14, RDT14, TZ11].
Characterization [DDP+18, VT14, XWSW13, CBP+15, DGL+13, GBW+14, GZZ12, Kop15b, MJBMI2, MPA10, RNP13, ZYG+14].
characterize [MGCC19]. Characterizing [LH11, PRSG13, She12, Yu12b].
characters [LSH+11, ZLL+10]. Charge
[CMF+17, JM11, RDT14, SFDE16, VV19, AWF+18, AS15b, ANH+11, ALH+10, BCSJCJ+13, BE16, CS14, CBTZ16, CMS13, Cor17, DS12a, DWR17, DAdeGR15, EFAC13, ENKK+17, GMG+10, HLWD15, JCGVPHT17, JZZM14, Kan15, KVR10, LLLMI1, LPE+10, LBDP12, MSV16, MCF+18, MRHR11, MPBJ11, NN18, OBW12, PL14, PTB+15, RSSG18, RO14b, Ric16, REL17, SPS+12, SFM+18, SSSG15, SmIN+19, SMP17a, SFLG+17, SLC+17, TN10, TKN10, UT15, UKG18, VPR10, VAR12, VL17b, WCT+11, WWCL15, YKO+11, YWZ14, YLZ+10, YJ17, YFH+19, ZDZM13, ZZL19, dLC17].
charge-assisted [SSSG15]. charge-inverted [UT15, YJ17].
Charge-transfer [JM11, ANH+11, EFAC13, YLZ+10]. charge-transport [HLWD15]. charged [BK13, KD10, MRO17, NPP13, RJS17, Tsi14].


chromophores [SGDT10, UD12]. CI [CME11, EFAC13, EFS16, FE14, IN13, KMS+19, MN19, PH10b, RSR+17, SCF+19].
circuits [RBV+12]. circular [HNNR13, SEJ+18, SB13, SB15]. circularly [SEJ+18]. Cis [CSM16, MSBF16, WvRSM14, ZLHH14]. Cis-
[CSM16, MSBF16, WvRSM14]. CISD [dALdS+15].
cisplatin [dRCFGRB18, CK17, PML+12]. CI

[ATP18, ASS+17, CXS10, EP+15, GPK+16, KKR+13, LDJ+10, LLL+11, LZJ+11, LGW12, PMG+16, Rab12, RVdMB16, Sak18, TFS+10, TFS+11, WGN+16, WGLG+16, YS13, ZCK+16, ZLLL12, CSNCS+18, JCG+10, JLS+10, JLH+14, LTL+15b, MSCP19, WHLZ12, WLF19, ZWY+10b]. Clar

Clusters [SC17, TT18, AFPI13, ATIP18, AF14, Ano11, ASS10, AC12, BPM15, BACSCI+10, CCL+13, CZZL19, DAI9, DH11, FCW+14, GT10, GC18, GRD+10, GAMAC+14, GZZ12, GBGR16, GBG+19, HS14a, HS16b, Hsu14, JM11, JCP14, JHMB+09, JHMB+11, JCG+11, KD10, KKPT11, KOP+14, KSNT19, KDB13, LZTV10, KL13, LZZ+11, LCH+15, LCWW10, MCS11, MPA10, MPA12, MP13, MBFG15, MBRC15, MCBY15, NC13, NC14, OKY18, PM18b, QZ10b, Rab12, RGVC+19, RSB+13, SN16a, SBGP18, SB11, SIT18, SMP17a, TN12, TNI+19a, Tak10, Tak11, Tak18, TSZQ12, TN19b, TS11, Tsu19, US11, WHL+10, WYGW12, WZH+18, YVEI+17]. CM1 [VSA11]. CN

[TS15b, YKH15, KIOY19, STS+10, TCPP14, WHDL11]. CNH [DBGO+17]. CNO [OKIS17]. cNOR [BS16a]. CO

[Bac10, BPLL12, FD16, FH+19, OKY18, SC17, SSX+14, YXZZ17, ZBB16, Spr10, WWKS16, BPLL12, CCJC10, DHE+12, DSHLM18, GLZ17, GWRJ18, HFSO12, HVS16, KD10, LLC17, LPLB16, MG15, MBFG15, SSC+19, SKTT11, WC13, AAMR18, CMM18, HYL+11, JCG+11, JWJ+10, YMY+19].
coadsorbed [LLTC12]. Coarse
[KZP+18a, MSLS10, NST14, BJP15, BLKP12, CAD16, GMPB12, HHWL17,
JC16, KCK+17, KVQC+11, KLS10, KMLS10, LZ12, LZX16, LZZ14,
LZLMP16, MT19a, MBC11, MBC13, ML14, RSG+10, SLX+15, SDZ17,
SOM+13, SJ17, SYG+18, SM15, SAvG15, WBF17]. Coarse-grained
[KZP+18a, MSLS10, NST14, BLKP12, CAD16, HHWL17, JC16, KCK+17,
KVQC+11, KLS10, KMLS10, LZ12, LZX16, LZZ14, LZLMP16, MT19a,
MBC11, MBC13, RSG+10, SLX+15, SDZ17, SJ17, SYG+18, SM15, SAvG15].
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[ZX11]. deiodinase [CFM+19]. delayed [FWS+18]. deleterious
[LX+11]. delineate [SBT17]. delocalization
[BK11, FV810, HSB+11, Jan16, Mat14, SS+13b, SSA+17]. delocalized
[Alg17, HSH15, dLC17]. DelPhi
[DLSA14, JLCA17, LLZA12, LPLA13]. DelPhiForce
[LCA17]. deltahedra
[LK16b]. deMon
[LZdL+10]. deMon2k
[BT10]. Denaturation
[IPAA11, FMG12]. Dendrimer
[MJBM12]. dendrimers [CAD16, HDHL15a, HDHL15b, HDHL15c]. Deng
[Ano12u]. dense [ASK18]. Densities
[ATM18, ATIP18, HGCCCGR+16, LP11c, MA16, REL17, UCRL18, dLC17]. Density
[AMK11, CD13, CWHH11, CKH19, FPV13, FD16, GMBM18,
GNGCA10, GWPJ11, INT18, JYS+12, KKPT11, LBGS16, LGW12, LLX+19,
LBTV12, LPMT17, MP19a, MWJ+11, MAP18, Oht16, PPH+14, RB12,
RSLML12, TS10b, UvSvdWK19, WDLG12, WGN+16, YJ11, ZLZ14,
ZYG+14, ZLY+10b, ZLY+10a, dSdS12a, ALK+15, Ali18, Ano15-59, AG12,
ASS10, BY11, BLBG+13, Ben17, Boz18, BBI+11, BZB+13, BG13, CHG+16, CRZ+18, CDB10, CR14, CAA10, CBO15, CC15c, CGR16, CKH17, CSXZ17, CC11, CAP17, CNK97, CPL11, CXD+19, CB11d, DAP+18, DH17, DWC17, Dl15, ED15, EP12, FED17, FCPJM14, GAI14, GHL17, GZL+12, GWJR18, GMG+10, GSS13, Gra15, GEG11, GAJ17, CHN19, CDB10, CR14, CAA10, CEBO15, CC18, CGR16, CKH17, CSX17, HH13, Holf14, HG10, HOK17, IKN13, IM17, JCP14, JLH+14]. density [JW16, KD10, KB10, KSSH13, KOP+14, KGHK12, KB13, KZ+16, KLN12, KYG+15, LL15, LRVM18, LCM12, LHKS12, LWG12, LH14b, LH17, LHZ+17, LK16a, MRC+18, MGL18, MHH19, MSY19, MCF+18, MGCC19, MAK+14, Mat14, ME10, MKM+17, MFR+17, MMJ10, NS18, NF17, NN18, NO16, NKK+16, NFI+16, NS17, OHPR18, ORZ11, OM12, OVPK15, PK17, Pie14, Pil17, PW12, PZM15, QZ10b, RJP12, RS13, RB13b, RSG14, Rod13, RHPWS13, RHT+15, RNS19, REV+17, Rui11, RSKG14, SPS+12, SGPJS+17, SH15, SSI6a, SDF+17, SFG+17, SHL+18, Sca10, SCW11, SDM+16, SEF+16, SE14, SH14, ST13, SHL+13, SPR+13, SXX13a, SXX13b, SMM15a, SMM15b, SMM+18, SXTT11, SZZS16, STS15, SK11, TldG+12, TN10, VGV+11, VAR12, VECT12, VV14, VV17, VED10, VHS+19, Vy16, WC10a, WHL+10]. density [WGL+11, WCUW11, WWU12, WWC15, WHX+10, WL14, WTH+16, XYW+14, YLZ+10, YS13, Yu12b, ZTH+15, ZXX+10, ZSWL12, ZKE+17, ZDX11, ZLHH14, ZCWX18, ZGS+10, dSdS12b, dSdLBNB17, dLC17, dLVoNC18a, CDM10, FAS+18, VV19]. density-density [JS16a]. density-fitting [Boz18, Hili3].

**Density-functional**


**Derivatives**

[KTSW11, CWHH11, CZH12, CBZ16, CROB16, HSZ+11, JS17a, JYS+12, KG11, KPT15, LWG12, LWG12, MFR+11, MIS+15, NS10, NF18, PC14, RVB+12, RFN15, REH13, SBR13, SX13a, SX13b, VV15, VV18, VSD10, WGL+11, WRG+17, WDP+12, Zsa10, ZW11, ZL12, ZWW11]. derive
MCK17a, MCK17b, NKJ16, NC12, NMLD13, PTK11, PHK14, QLYL10, RS17a, RDF+11, RS14, RRC+15, RLZ+18, RN17, REL+17, RKB+14, RK15, SRF+17, SWM10, SCF+19, SRL+15, SDL14, SZ+18, SPZP18b, TNI+19a, TSNC+17, TG12b, Tsi14, TS15b, Tsi17, VVJ15, VECT12, VAMS14, WKLC12, WYGW12, XKW18, YZGS14a, YZLZ19, YSRSS10, YZ15b, YXZZ17. DFT [ZCK+16, ZWGO12, ZZWT12, dSDdAR10, vS18]. DFT-based [NKJ16, NC12]. DFT-derived [REL17]. DFT-MD [GMASBF16].


dihydroxylated [LDH+14]. dihydrated [HvM19]. dihydro [RS17a].

dihydrofolate [RKDM14]. dihydrogen [PM13, UT14, WHX+10].

dihydrogen-bonded [UT14, WHX+10]. dihydrogen/hydride [PM13].

dimension [HKRS11]. dimensional [BPLL12, FBvdB18, FZL+19, KYT+17, KRSC12, KTO13, MB16, PJ13, SG10a, SHL19, TYN15, TCX+13, TKC+11, XCLZ19, YZLZ19, ZWX16].
dimensionless [MS10].
dimensions [CHC+13, HAL14, SRL+15].

dimer [LWL+16, ARRC15, ANH+11, BPPS17, CBTZ16, FCL+10, FMNC11, JT18, KB1+12, LCB10, Nav18, PD11, SKY+11, Tac17, WWKS16, YCGA10].
dimetric [PS14].
dimerization [DSD+11, KAR12, TNI+11, ARRC15, ANH+11, BPPS17, CBTZ16, FCL+10, FMNC11, JT18, KCB+12, LCB10, Nav18, PD11, SKY+11, Tac17, WWKS16, YCGA10].
dimerization/oligomerization [KAR12].
dimers [AM19, BCNH+11, BWKW10a, BWKW10b, CLFRO18, CK10, DT19, JKS+16, LJW11a, LMI+14, PG18, PVS12, RS13, SZZS16, VT14, Zha11].

dimetallic [ZYG+14].
dimethyl [GC11, KPH+19, WLC12, ZSWL12].
dimethylacridine [FWS+18].
dimethylaminoazobenzene [KP10].
dimethylaminophenyl [YLZ+10].
dimethylnitrosamine [FFA14].
dimyristoylphosphatidylcholine [ML14].
dinitrophenol [MIS+15].
dinuclear [ITY+19, OSS10, QLYL10].
dioxane [GM17].
dioxetanone [RSLML12, dSdS12a, dSdS12b].
dioxide [SC17, KPH+19, Kop17b, QZ10b].
dioxygen [DSM+11].
dioxygenase [DGH+11].
dipeptide [EJ13, IO13b, LL19, MAMF19].
dipeptides [DHF+11, RSL16].
diphenyl [GKR13, Ray13, RKG11].
diphenylalanine [KLN16].
diphenylamino [FWS+18].
diplatinum [KT12].
dipolar [YZN13, CSS17, AKM11].

dipole [Ali18, GH16b, LIRL+16, ZBG11, AS15b, BLBG+13, DHOG13, GH16a, HBKL10, IY18, KCB+12, LHHW14, MNNK10a, MNNK10b, PC14, Yan11].
dipped [IN13].

diradical [HWWB19, VSH19, YSSB12, ZB18].
diradicals [SH18a].
direct [LZY12b, SM18, WAM17, FF11, FSSW17, FZL+19, JCG+10, MMH19, RSB+13, Yu12a, LLHM16].
directed [CH14, HBBY10].
direction [PAK17].
direction-dependent [PAK17].
directionality [WGD+16].
diruthenium [CRC13].
disaccharides [GMSV14].
discharge [SMiN+19].
disconnectivity [SOJ14].
discotic [AWF+18].
discover [Hsu14].

Discovery [AKMT11, Aki16, CF18, FMG12, HYYYZ13, Ibr11, IGK16, PVJ10, RRV+18, Zim13].

discrepancy [Yan11].
discrete [EJ13, MCUJ15, WAM17].
discretization [AD10, LLFH16].
discriminate [UCFR16].

Discriminating [FZL+15].
discrimination [YL13].
discriminative [KS12].
discussion [CDB10].
disjoint [BK13].
dismutase [GEP+14].
disorder [LLL+12].

Disordered [MYT18, GP12, LC16, LC17a, NDLW13, SJZ+15, ZC14].

Dispersion [HSJ18, AG12, BCNH+11, CLFRO18, cCVG+14, DAG19, GEG11, Han11, Has14, HGHP14, ITIN15, KB10, KSSH13, LCM+14, RJP12, STS15, SB11, SB13, TG12a, WM17].
dispersion-corrected [CLFRO18].

Dispersive [TG12a, SDB+16].
disproportionation [DLP11].
dissected [FNSF+11].

Dissecting [CLFRO18].
dissection [BMFG16].
dissimilarity [HS17a, YDL+10]. dissipation [VVG13]. Dissipative [PH17, SCK18]. dissociation [CR19, CCJ+11, GCCM15, Gil11, LBC+12, LL10c, MH11, Rob13, TNY18, WSH10, Won18, YPvD13, ZWLX11, ZZZ19].
dissociative [HBL12, RIJ+11]. dissolve [SG10b]. dissolved [SIG+15].
Distance [PHDH13, DCS15, Hug14, JMS13, KCPMG12, LZ12, PUPGD10, RPNP10, RRH12, UT14, You16, ZT14, dACP12]. distance-dependent [KCPMG12].
distance-dependent [VVG13]. distance/interaction [PH17, SCK18].
distance/interaction-activation [PH17, SCK18].
Distinct [JAMS+19]. distinction [ZY14].
Distinguishing [FD14, GMBX+16].
distortion [INT18, LSL+19].
distortion/interaction [LSL+19].
distortion/interaction-activation [LSL+19].
Distortion [KCPMG12].
distortion [INT18, LSL+19].
distortion/interaction-activation [INT18, LSL+19].
Distributed [XFG+16, BMBJ11, KNR+18, UIW+10, XFG+15].
distribution [AS15b, BCSCJ+13, GWF11, GMG+10, LRER13].
distance [PHDH13, DCˇS15, Hug14, JMS13, KCPMG12, LZ12, RPNP10, ˇRRH12, UT14, You16, ZT14, dACP12]. distance-dependent [KCPMG12].
distance [VVG13]. distance/interaction [VVG13].
distance/interaction-activation [VVG13].
Distributed [XFG+16, BMBJ11, KNR+18, UIW+10, XFG+15].
null
GBG\textsuperscript{+19}, HTY\textsuperscript{+19}, NNT\textsuperscript{+19}, THP\textsuperscript{+15}. Efficacy [LC17a]. efficiencies [RO14a]. Efficiency [AC11b, BB11b, BB11c, FE14, GBSE11, XFG\textsuperscript{+16}, AC12, GSHM10, LY10, LWL\textsuperscript{+11}, LZZ\textsuperscript{+15a}, MKGA10, RO14a, XFG\textsuperscript{+15}, vLBBR12]. Efficient [AB16a, BC13, BAS14, Cas13, DMAH15, DBF14, EP10, GCWS15, GPK12, Ham11, HNS16, HDL\textsuperscript{-14}, HHWL17, JMS13, KNR\textsuperscript{+18}, LZ11, Les19, LGKS17, MKS\textsuperscript{+12}, NYN17, PSS14, PAK15, Ran12, RJS17, SS16b, SSP19, TJB12, UCRL18, WHAS\textsuperscript{+16}, WM12, ZZ14, ZKE\textsuperscript{+17}, AM10, BW11a, Boz18, CBP14, CHG\textsuperscript{+16}, CY09, CY13, CZZL19, CMS13, DS15, DGL\textsuperscript{+13}, GREA11, GWZX12, HDL\textsuperscript{-17}, ISK14, JZ17, KB11a, KKH18, KV15b, LFB14, LPK16, LLZA12, LZZ\textsuperscript{+15a}, LZ11, Les19, LZS\textsuperscript{+17}, LAS\textsuperscript{+14}, NPTS16, NF18, NN18, OK16, PW12, PBG17, Ran13, RR14, Rod13, RSL16, SCQJ13, SA13, SMBW09, SCSW13, SWB\textsuperscript{+12}, SUN5, TO10, WJC\textsuperscript{+13}, WOH18, WLQ19, ZWP11, Zha12b, Zha12a, vLBBR12, WHAS\textsuperscript{+10}. Efficiently [WES13, ASMS10, DDK14].


Ehrenfest [Dil15, FED17]. eigensolver [KZZ\textsuperscript{+16}, KCC\textsuperscript{+18}].

eigenvalue [Coh18, HLXH17, HLXH18, eigh [HDK\textsuperscript{+12}]. either [TCPFC14].

elastic [ECZW17, LBTV11, QB10, QB11, SH11a, XTY\textsuperscript{+14}]. Electric [GH16b, LL13b, B LFZ13, B LBG\textsuperscript{+13}, BS10a, CXS10, GH16a, KZK\textsuperscript{+12}, MRB14, PdSC18, SH15, SLX\textsuperscript{+15}, Yan11, YJ11, YCK16, ZSL17].

electrical [LLLM11].

electro [TMJ15].

electro/nucleophilicity [TMJ15].

electrochemical [SKGP19, SIG\textsuperscript{+11}, SGH\textsuperscript{+16}, YJ11].

electrochemistry [DSK17].

electrode [MKO\textsuperscript{+13}].

electrodynamics [Tac19].

electrolyte [KS18].

electrolytes [HAL14].

electrolytic [SV11].

electromagnetic [SEM12].

Electron [BK11, Bar14, BLG11, BKW\textsuperscript{10a}, BKW\textsuperscript{10b}, CBO15, HS16a, HRMAL\textsuperscript{+13}, HGCCGR\textsuperscript{+16}, KGR\textsuperscript{+16}, LLX\textsuperscript{+19}, Pil17, VV19, WWU12, ACD\textsuperscript{+13a}, ACD\textsuperscript{+13b}, ABGN12, BH12, BT18, CDB10, CAA10, CWH11, CC18c, CJPTC18, CTP13, CXD\textsuperscript{+19}, DA1G\textsuperscript{+15}, ED15, EP12, ES\textsuperscript{+12}, EP15, FROS14, FWS\textsuperscript{+18}, FED17, FCPJM14, GNDA\textsuperscript{+12}, HSH15, HPT17, HEMCZE\textsuperscript{+14}, HAP\textsuperscript{+12}, HBL12, IYK11, Jan16, JBSQG11, JSS19, KPL13, KTK17, KKA\textsuperscript{+18}, KYG\textsuperscript{+15}, LW16, uLhY11, LRMV18, LHO17, LYL16, LLJ12, LP11c, MRC\textsuperscript{+18}, MKGA10, MRB14, MT19b, Mat14, MBFP15, MKH\textsuperscript{+13}, MCK17a, NYH\textsuperscript{+17}, NLL19, NS17, PAK17, PGdO\textsuperscript{+16}, PSC11, PS17, PT16, PHT17, PC16, Ras17, Rod13, REL17, RSKG14, SF\textsuperscript{+18}, SZB19, SB14, SHB17, SHG13, SK11, SSA\textsuperscript{-17}, UCRL18, VGG\textsuperscript{+11}, VC12, V17a, VCL18, VI17, Vy16].

electron [WLW\textsuperscript{+10}, WMW11, XBBS19, YK10h, YLL11, ZPP\textsuperscript{+16}, ZCWX18, ZGS\textsuperscript{+10}, dLC18a, dLvNC18a, GBM18, SDIP18].

electron-correlation [NYH\textsuperscript{+17}].

electron-deficient [YLL11].

electron-hole [PTB\textsuperscript{+15}].

Electron-pair [WWU12]. electron-sharing [JSF19]. electron-vibrational [CJPTC18].

electron-withdrawing [CWH11].

Electronegativity [FCJM14, vS18].

Electronic [AMQ\textsuperscript{+14}, AM19, ASS10, BAD\textsuperscript{+19}, DA1G\textsuperscript{+15}, DGSSVGM19, GNDA\textsuperscript{+12}, GNI18, HLW\textsuperscript{15}, Ibr17, KYCL11, KKL\textsuperscript{+13}, LLBO12, LS11b, MT19b,
MP19a, MAPB10, NIIT15, PMC+17, RLA+11, TN12, TNI+19a, TN10, TFQ+10, TS15b, VI17, WRM+12, YW12, ZRCC11, AR15, AK10, AC12, BLZ+13, CPRS18, DKE+17, DHOG13, DMD+18, EVR18, EH13, EWK+13, EBP17b, FB10, GRR10, GRARO+14, GXW+12, GZZ12, HASR+12, HS14a, HSB+11, HuA16, IEF+10, KKH19, KPT11, KSM17, KG11, KKA+18, Kop15b, Kos16, KP10, LGOM+15, LX11, LBT11, LBT12, LXZ+10, LSH+11, LLW14, MC10, MA16, MCF10, MCF+18, Mat10, NC14, NS18, NCT18, NFI+16, OLA15, PdSC18, PKH14, PTB+15, PVAM16, Pyy13, RCa+13a, RML+15, RR12, RR11, SFA17, SLP+12, SIT18, SRS14, SB15, SKGB13, Tac19, TFQ+11, TD10, TS15a, TNG+10]. electronic
[TS11, TG12b, Tsu19, TEDT18, VVP12, VHR16, VAR12, VBMA13, VLGK+17, VGTL16, WGL+10, WGL12, WJG+13, WO15, WSGN11, WXK+13, YK13, YFH+19, ZJZM13, zZb111, ZBB16, ZZZ+19, dCDP15, dVAG16, vSGP10, LKZM18, SZL19]. electronically
[BSL16, LSH+11, LYSS11, RIJ+11, SFCCK+14, SFCCK+15, YB11].
electronics [RN17].
electrons [EKH14, FHZA+18, WCY+11, WRG+17, Xhd15, YCGA10, Sah18, SGP18]. electrophilic [MA16, WDS+19]. electrophilicity [YB16]. Electrostatic [CLA16, LP11b, MLZZ12, Sch18, WFZ+18, ALRM18, AS18, BT18, BCNH+11, BSF18, BK13, CCC+11, CS14, CPK12, CB11c, DLSA14, ER18, GBL+11, HOK17, IO13a, KTNN10, KYG+15, Lr11, LCA17, LCM16, Mat14, NF18, OHR18, PV10, RB13b, TY10, VSMR+17, VV18, YKO+11, YWJ+16, YAO18, YMP14, YZL+15, ZDZM13, ZBP11, KGM12].
Electrostatics [BSG18a, CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NLP+16, SDZ17, SWPR11, UHH+11, XXY17, YMP14]. element [BCCO10, GPK+16, RMGB11, TG12b, TCX+13, XXY17].
Elongation [OLA15, MKGA10, MKGA10]. Elongation-MP2 [MKGA10].
Elucidating [HNHR13, TDP+12]. Elucidation [CPLL11, TNYN16].
embedded [DSF17, GMG+10, HSH15, ZFS18]. embedding [CCB15, ESD18, ESM+12, HH16a, HH17, Höf14, HOK17, KSR17, NF18, NOKJ16, RR12, SDF+17, SS16b]. Embelin [CPR18]. emerges [MNK10a]. emission [CSC+18, LX11, LMCd10, PLP+16, SGWA17, WDP+12, ZLL+10].
Enantioselective [ORZ11]. enantioselectivity [OAN15b]. encapsulated [EOO+16, STS15]. encapsulating [WZH+18]. encapsulation [YDGZ15]. encoded [RSL16]. encoder [LDH+14]. end [HDL+17, SL10]. ended [RJR14, Zim15]. endo [FB14a]. Endohedral [NKD18, FL15, MCK17a, MCK17b, ZSL+11, ZYG+14]. endohedrally [NKD18, FL15, GLF16, MCK17a, MCK17b, ZSL+11, ZYG+14]. endohedral [JKH18, YTS+18, BB11a]. Endo [GRCL12, FB12]. enediyne [DCHL12]. Energetic [JCHT18, JW12, CG15, MCAG+16, MvBD18, PBG17, SB18, SLHW09, TPL+10, YRSS10, ZZWX11, ZYL+12]. Energies [AF14, AS14, AG12, ABS+19, BW11a, BLF14, BVHI17, BS16b, BE16, BS18, CHG+16, CMD13, CR19, CH10, CTP13, CXD+19, CBG16, DHO13, DMJ17, DHH+11, DPOS16, FGM11, Gil11, GP11a, Grl13, HAK+10, HH10, HH11, HLM+17, HHWL17, IK13, KS13, Kar17, K15, KDE12, KB11b, KPY13, LHW11a, LW11, LHWW14, LH14a, MCS11, MS13, Min18, MS12, MBE16, MMJ10, NW17, NMF+14, OB12, yOTn16, OAN15a, OS16, PGCT+12, PP14, RLD+17, Ran19, RDDS10, RAR+11, RO14b, RZ16, RR14, Rob13, RJ17, S12, SHL+13, SOD+11, STM+15, S15, TS16, UD12, VVG13, VECT12, VM11, WBT10, WS10, WJ+13, WGA18, WGI2, WX12, YAS13, YMP14, ZZ14, dALdS+15, dBO13, NQB19]. Energy [DK11, GS16, IHY15, JCGVPHT17, LFN+10, LPLB16, MYKO18, OSI+19, PK19, SN16b, SSGS15, Spr18, SKGB13, WM12, AMGB10, AC11a, Ano10a, AK10, AK16, BSC+13, BPM15, BRE16, BH15, BS16a, BRLS08, BL12, BCSC+10, BG17, Bon14, Boz18, BD11, BWMS10, BB11b, BB11c, BG12, CM13a, CK10, CDM+15, CLA16, CY09, CX10, CY11, CY13, CH16, CSXZ17, Che17, CF18, CS17, CHR+12b, CHR+12a, CP10, CMv10, CP12, CWZ10, DGH+11, DWR17, DB11, DS12b, DH14, DWC17, EV14, FMNC11, Fer17, FED17, FC12, FCOG12, FSSW17, FCCP17, FL11, GS14, GS15, GHK12, GO13, GNO16, HNY19, H+17, Hel13, HDM+15, HH15, HG13, HMY16, HYUS11, HJ13, HG18, HYD10, HDHL15a, HDHL15b, HDHL15c, IMK+16, ISN13, JCP11, JML13, JZ12, JZZM14, JXC10, KB+12, KTT16, KB10, KIO19].
SC18b, SBN13a, SBN13b, SOvG12, SLG15, SNS13, SN10, SHB17, SMM15a, SMM15b, SMZ+18, TM18, TSN16, UCFR16, UGK18, VLB+10, VT14.

energy [VGV+11, VLI7a, Vyb16, WKC+10b, WLF11, WSH10, WGL+11, WWW18, WZ19, WHM10, XHLH16, XYW+14, XFX+16, XVN17, XCLZ19, YOMT14, Yan14, VLB+10, ZPF14, ZLT13, ZH12, ZSB+16, vLBBR12, NK19, SGP18] energy-adjusted [HH15]. enforced [BW11b].

dm [BEFS13, DBDP16, HC14]. engineering [KLZ+18].

enhancement [CFC15, HTS15, IMK+16, KvdV14, SSO19, Bou14, CF18, KKO+16, KJM+17, LC16, MBFG15, SLLL13, ZLM+15].

enhancement [LLL+11, MA17].

tenaltic [HBR17].

enterprise [WDY13].

enthalpies [cCVG+14, HFK+12, LLH11, LWL+10, MRR11, SHL+18, WKC11, WDW12, ZWLX11, MSPC19].

enthalpy [UGFR16, vADC+14].

ten[CHR+12b, CHR+12a, Pro16].

entropy [BMPML+13, HUG12, LLH11, LWL+10, MRR11, SHL+18, WKC11, WDW12, ZWLX11, MSPC19].

entropy-based [BMPML+13].

environmental [GMG+10, GCC14, HS16b, LGVA14, SIG+11].

enzymes [GH10, LT13, RIJ+11].

enzymes [HH11, CQFC10].

EOM [KK17a, KKL+13].

EOM-CCSD [KK17a, KKL+13].

EPIC [TNG+10].

epidermal [BHF+18, WC11].

epidermis [CGBK13].

epitope [GRP+12].

epoxidation [WCDM11].

epoxide [DSHM18].

epoxides [BCP+10].

epoxy [HTY19, LPMT17, PPH+14].

epoxy-carboxylic [LPMT17].

epoxy-phenol [PPH+14].

equality [ABS+19].

equalization [vS18].

Equation [NNT+19, AA18, BCCO10, CD16, CLA16, Fer13b, Fer13a, FCE15, Fra15, Fra16, FC18, KS18, KK17b, RSLS13, SK15a, SM16a, SG10a, WBVE16, XYX17, YS18].

equations [BYE+16, ZR10].

equilibrated [WHAS+10, WHAS+16].

equilibrating [OPR16].

equilibration [LBDP12, SMP17a].

equilibria [GWJR18, LC17b, PHH+16].

equilibrium [DSF+11, FD14, LLvG10, Lvg13a, MCLD10, NHHN16, SJWE10, WXY14].

ergodicity [KCK+17].

Erik [Sch10].

ERKALE [LHSH12].

Ermod [SM14a].

Errata [CHR+12b, HRJ+15].

Erratum [ACD+13a, Ano15-59, Ano15-58, Ano17-35, ABB+13, BRSL12, CY13, Fra16, GLW13a, HNWF12, HvM17, HDHL15a, HDHL15b, HLXH18, ICS+13, JHMB+11, Li14a, MSK+12, RK16a, SFCCK+15, SBN13b, SZX13b, SMM15a, WHAS+16].

error [HAGK10, Hua16, KFT18, PHH14, PD11, WNP+16, ZH12].

errors [LEdOLLV17, vS18].

erythrose [SM17].

ESCF [vW11].

esculetin [LYSS11].

ESES [LWZ+17].

eSHAFTS [HSW+19].
[DWR17, RF15, KB11b, TTB+11]. Estimation
[RLDJ17, ABS+19, BPE16, CZY11, Fer17, GLM+17, HHL17, Hug14,
JKS+16, MSV16, MRR11, OZS+13, PHK14, SY11, TM18, YOMT14, ZH12].
Estimations [RLA18]. estimator [FCPJM14, WBF17]. etching [KHE+19].
ethane [Tak11, ZLT13]. Ethanedithial [SMB18]. ethenol [AAMD+11].
ether [HLB15, WLC12]. ethers [GKR13, Ray13, RKG11]. ethylene
[KCB+12, KT12, LL13a, MCC11, SFM14, TLA10, XZ11, YMY+19, SMB18].
Etomica [SK15b]. ETS [CSM16, DBGO+17]. ETS-NOCV [CSM16, DBGO+17]. Eulerian
[LWZ+17]. eV [KKH19]. evaluate [BY11, KPL13]. evaluated [VECT12]. Evaluating
[DKE+17, Sch18, SJ16, WGIz, HLS12, JLS18, VLI7a, XSZL11]. Evaluation
[AYYO17, CHR+12b, CHR+12a, EP12, HG10, LLC+10, MBE16, MCK17a,
RRH12, RB13b, WNM17, YD17, BMRI11, BLPF13, BLF14, DLT17, DS12b,
GS11, HBI+17, ISO+13, KLOS10, Kos16, KT18, KSC16, LW11a, LW11,
LHW14, LZY12b, NN18, PW12, SF18, UM13, VBD5+11, VM11, WO15,
PLAG11]. evaluations [HP10a]. evaporation [RSB+13]. event
[BSL11, HNS16]. event-driven [BSL11]. events
[LSvE17, Luv12, ONTTL16]. evidence [RS17b]. Evolution
[RSGK14, WCY+11, CJI+13, GAMAC+14, MGCC19, NGA17, Niz13,
YHI+13, Yes15]. evolutionary [BDdS13, CDS16]. evolving [SL17]. Ewald
[AG11, NO16, YWJ+16]. EX [PMG+16]. EX3 [GPK+16]. Exact [BKLA13,
GREA11, RP15, dLC18a, BSZ+12, BTB+11, KTSW11, LLZA12, Vy1b5].
exacting [BS10b]. Examination [DT19]. example
[BBG+18a, GREA11, MS15, RRR16]. Examples [HJG09, LK16b]. EXAT
[JCGM18]. ExcelAutomat [LSL+19]. Excess
[LLX+19, WILW+10, Fra15, Fra16, WCY+11, YCGA10]. Exchange
[CKH19, DAB16, GS16, Ru111, XFG+16, ZLZ14, BTB+11, CSKH15,
CSKH16, CCH17, CQPP11, CH16, COOH14, CAT+13, ENKK+17, GS15,
GW+12, HG10, IYK11, IHI+13, KCK17, KTO11, KTO13, KCL+14, LPAS11, LC17a, LL11, LMI+14, MC10, MS16, OGL10, OLI3,
OLY17, OZ14, PW12, RFH10, SH18a, PH11, SH19, SNB13a, SNB13b,
SH18b, SA+17, TK11, VL17a, Vy1b5, Vy1b6, WY17, XFG+15, ZC14].
exchange-correlation [HG10, SH18a, Vy1b6]. exchange-coupled
[CAT+13]. exchange-repulsion [CGPP11, ENKK+17]. exchanged
[DAP+18, LZTV10]. Excitation [KDR+18, CHG+16, EFAC13, Les19,
MEH18, PTB+15, SHB17, TG12b, TSN16, UDI2, WJG+13, WZ19, WGA18].
excitations
[ACD+13a, ACD+13b, CMF+17, FE14, IIF+10, PVAM16, WWD14, XTn18].
Excited [CH10, FHG+19, SGWA17, ZZS+10, BSL+16, EK17, ESM+12,
FD14, FAA15, FD16, GA18, HNW07, HNW12, HH17, HZS17, HDHL15a,
HDHL15b, HDHL15c, JCGVPT17, KT19, KPG18, KB14b, LLBO12,
LLW12, LWW12, LWG15, LGC19, LX1, LSH+11, LYSS11, MPG11,
Excited-State [FHG+19, SGWA17, FD14, GA18, HH17, HZSS17, KT19, LWGZ15, MPSG11, NYN17, PH10b, WHL+10, WHX+10, YD17, YHX19, YLZ+10, YB11, YYT12, L2Z+10, PGW17].

Excited-states [LLBO12].

Exciton [HRH+17, LSH+11, SEJ+18, WZ19, ZSL19].

Exciton-phonon [WZ19].

Excitonic [JCGM18, LCK+18, ZMMM12, NNT+19].

Excluded [LWZ+17, Yan14].

Exclusive [dLC18a].

Exhaustive [DKV18].

Existence [BMB13, WD10, NKD18].

Existing [KT18].

Exothermic [LWL+16].

Expand [BK17c, Car14].

Expanded [MLQ+12, TSNC+17, YSSB12].

Expanding [GMZ12, UCRL18].

Expansions [HAGK10, HSN14, LYC+13, LRER13, NF17, SS16a, SNS13].

Expected [Clo15, AF14].

Expedited [DJD12].

Expensive [LDZW17].

Experiment [GNC+18, JAH+17, SA10].

Experimental [MRC+18, NHF+10, AvKSP16, BRGN12, DCD13, EOO+16, GpD+16, HJ13, KP10, Pog10, RO14a, SB10, SGS+16, SKMS13, VZ14, CYI+10].

Experiments [CBP14, HCB11].

Explained [FL15].

Explicit [WG14, BEM14, CC0H14, CBG16, EK15, ENK+17, GLB16, HDL+17, KJD12, LH11, RDA12, SYH12, SKMS13, Zha12b].

Explicitly [yOTn16, SM17].

Exploiting [HB14, BYE+16].

Exploration [FHG+19, OSI+19, ZGS+10, BGL+18, CF18, LW12, LAW+16, NLR18, OKIS17, OKY18, RDC16, Sti15].

Explore [JPC11, MSC+10, MCC12].

Explored [WLF19].

Explorer [SYN+12].

Exploring [BHB12, BPPS17, BCG10, DSHLM18, MTM14, P13, Tsi17, VHS+19, ZST18+18, ZT14, dSLBNB17, RDC16, NOKJ16].

Explosion [GC18].

Explosive [YPC+10].

Exponential [BBOB16, BB11b].

Expressions [Gav12].

Extended [GWZX12, KUDG12, LRvdSM15, SSWX14, TSN17, YB16, Pon11].

Extending [LMZ11a, Man13, TTN19, VBV13a, VBV13, P HI+12].

Extensible [GCW14, JYC+16, LAS+14].

Extension [AIQ19, HSN14, PFVL14, SDZ17, VVW+18, YHVM12, Cam15, LL11, RLL12, RAS17].

Extensions [NYH+17].

Extent [GFGS18].

Exterior [HL19].

Exterior/interior [HL19].

External [GS14, PdSC18, SEM12, XTN18, ZSL17].

Extra [PFAS+19].

Extract [MDTD16].

Extrapolation [CC11, Lyc+13, OAN15a, SRR16].

Extraction [CVG14, UvsdWK19, VVG13].

Extrapolation [CC11, Lyc+13, OAN15a, SRR16].

Extrapolation [CC11, Lyc+13, OAN15a, SRR16].

Extremely [ZM11].
friendly [DBF14, SFR+11]. frontier [MGS+16, TZ12]. frozen [BVC13, Fer13b, Fer13a, HH16a, HH17, Höf14, SDF+17]. frozen-density [HH16a, HH17, Höf14, SDF+17]. fructose [RAR+11]. fructose-1 [RAR+11]. fuel [SV11]. Fukui [BVC13, PRY1+17, SBR13, YVEI+17]. Full [STM17, ACD+13a, ACD+13b, BPLL12, PS17, TSC+13, XCLZ19, dSdAR10]. full-dimensional [XCLZ19]. full-pivoting [PS17]. Fullerene [Avd18, NKD18, GKSS14, KCK+15, KP10, LTR18, Oht16, TPL+10, TFQ+11, TTB+10, XFTW15, YDGZ15, ZSL+11, ZZ12, SWA13]. fullerene-based [TTB+10]. fullerenes [GZH10, GLF16, MCK17a, MCK17b, SWA13, STS15, WTH+16]. Fullrmc [Aou16]. Fully [AG12, NLL19, ZSTI14, FBY+17, GBL+11, KG13, LZZ+13, Pop18]. fulvenes [AS18]. Function [GBMB18, ABDGN12, AB16b, BLGI11, CKP10, GS14, GND+12, GEG11, HH16a, HBL12, HYM16, IY18, JLCA17, JMS13, Kop15a, LL13a, LGH11, LCB10, LIR+16, MLG18, MB16, yOTu16, ON14, PiL17, PRY1+17, RZG+13, RvL11, SS16a, SFG+17, SK18, TCB16, TO10, UM13, UCPR16, WO15, WDHZ13, YVEI+17, ZLT13, ZCWX18, vSGP10]. function-based [WHDZ13]. function-guided [YVEI+17]. Functional [CKH19, FAS+18, FPV13, LLX+19, MP19a, AMK11, ALK+15, Ali18, Ano15-59, AG12, ASS10, BY11, BLBG+13, BK17b, BZB+13, BG13, CHG+16, CRZ+18, CR14, CWHH11, CSKH15, CSKH16, CKH17, CSXZ17, CC11, CNK97, CPLL11, CB11b, DAP+18, FD16, GAI14, GHL17, GZL+12, GNCA10, GSS13, GEG11, GJ+17, GWJP11, Han11, HDL+17, HNWF07, HNWF12, HPT17, HG10, HZSS17, INT18, IKN13, IM17, JCP14, JLH+14, JW16, JYS+12, KD10, KKPT11, KOP+14, KGHK12, KB13, KZZ+16, KN12, LCW12, LBGS16, LGW12, LBT11, LBTV12, LHKS12, LH14b, LH17, LPM1T7, MMH19, MSY19, MAK+14, MWJ+11, MAP18, MFR+17, Mor15, MMJ10, NS18, NF17, NN18, NO16, NK+16, Oht16, ORZ11, OM12, PAK17, PPH+14, Pie14, PD11, QZ10b, RJPB12, RS13, RB12, RSLML12, RHPS13, RHT+15, RNS19, Rui11]. functional [SPS+12, SH15, SFG+17, SML+18, SCW11, SB17, SEF+16, SE14, SH14, ST13, SHL+13, SPH11, SH19, SMM15a, SMM15b, SMM+18, SKT11, SZZ16, STS15, TLDG+12, TG12a, TS10b, UvSvdWK19, VV14, Vik11, VL17a, VI17, VLGK+17, VED10, VHS+19, WKL+10, WCW11, WDGL12, WYT17, WHX+10, WL14, WTH+16, WGN+16, XYW+14, YJ11, YLZ+10, YS13, ZXS+10, ZWLX11, ZSWL12, ZLZ14, ZYG+14, ZYW+10b, ZYW+10a, ZLHH14, ZG+10, dSdS12a, dSdS12b, CK19]. functional/basis [PD11]. functionalities [KAG+12]. functionalization [WWTL19]. functionalized [KYKR15, LdSRR16, LTR18, MSY19]. functionals [Ben17, CCB15, CGR16, CXD+19, DH17, DOM+11, DWC17, FPR114, GWJR18, HG10, HBI+17, KB10, KSH13, KSSH13, Kar17, KM13, LH+11, LH14a, LKB16, PW12, RSG14, Rui11, SGPJ+17, Sea10, SDM+16, SH18a, SPR+13, SZX13a, SZX13b, VCL18, WYT17, Yu12b, ZTH+15, ZWX19, dSdB17]. functions [BP18, BLZ+13, CD13, CC11, CVG14,

YVEI’17, LMA15. **GenIce** [MYT18]. **GenLocDip** [GH16b]. **Geo** [DLSD13]. **Geometric** [MK11, AM19, CDB10, CDBM11, EH13, FXC+13, HHT+13a, HHT+13b, LLFH16, REH13, TCC+13]. **geometric-quantum** [CDBM11]. **Geometrical** [DPAB16, HRJ+14, JRSHP14, LCM+14, SPR+13, Tak10, Tsu19, UT14, HRJ+15]. **Geometrically** [RIJ+11]. **Geometries** [Alg17, HCP15, SRA17, SIT18, Tak10, LXZ+10]. **Geometric-dependent** [EPD+10]. **Germanium** [GSMM15, ALH+10, Kop18]. **GeSbTe** [NIIT15]. **GFP** [UD12]. **GGA** [BG13, EH13]. **Ghost** [CMF+17]. **ghost-hunter** [CMF+17]. **Giant** [JCG+11]. **GIAO** [PTK11]. **GIAO-CCSD** [OPR16]. **Gibberellin** [HYYZ13]. **Gibberellin-binding** [HYYZ13]. **Gini** [WF16]. **GIPAW** [SPZP18b, SPZP19]. **Give** [AA18, JT18]. **Glass** [GFGS18]. **Glasses** [You10]. **Global** [LzDH13, OKIS17, PRSG13, Tak10, BK17b, CPN+17, CZZL19, DS15, DMAH15, GPE13, LK11, LL11, MP13, MB14, MO15, MCAY15, SKKS13, SC15, TszQ12, Vor10, WDHZ13, XhD15, XCLZ19, ZL11, DH11]. **Glu** [EJ13]. **Glucopyranose** [HH10]. **Glucosamine** [ZBP11, ZP13]. **Glucose** [APY+16]. **GLYCAM06** [SA10]. **GLYCAM06/TIP3P** [SA10]. **Glycan** [JSD+11]. **Glycine** [DB12, DP15, FCD10, MC10, SPZP18a, SPZP18b]. **glycoconjugate** [LABSG17]. **glycol** [MSY19]. **glycoproteins** [JSD+11, PFVL14]. **glycosaminoglycan** [CHKR10, SA10]. **glycosidic** [HH11]. **Glycodelin** [HPP+12]. **Glycosyltransferase** [RN17]. **GmbH** [Spr10]. **GMCT** [U12]. **GnomeoSim** [LWK+14]. **Gold** [Ano15-58, BH14, CCJC10, FHT+15, GAMAC+14, Li14a, Li14b, LHKS12, LH14b, MFR+11, MG14, MBFG15, SRR+16, SKTT11, YLL11]. **Gold-thiolates** [FHT+15]. **Goldberg** [WTH+16]. **Good** [SB10]. **GPCR** [LLHM16, MFR+17]. **GPgpu** [UM13]. **GPR119** [HK18]. **GPU** [AKK+16, AGB13, BK17c, CVT+11, DZT11, HAP+12, Kan15, KGHC15, KP+15, ML+18, MEH18, PZCL16, REV+17, SBV10, SOM+13, UTM11, YLGX14, YSG12, ZLL+13]. **GPU-accelerated** [AGB13, CVT+11, HAP+12, YLGX14, ZLL+13]. **GPU-based** [KGHC15]. **GPU-enabled** [BK17c]. **GPUs** [GBL+11, HLW+17, HLEM18, KK17a, RSRR15]. **Gradient** [DS15, CDM10, HHBY10, KN17, MN19, SH15]. **gradient-directed** [HHBY10]. **Gradients** [GP11a, WM12, Boz18, BWMSM10, CCB15, HH16a, HH17, LBGS16, LFN+10, RSG14, SFG+17, SSMW09, SLG15, TSH+19, vLBR12]. **grafting** [KKR+13]. **Grain** [SOM+13]. **grained** [BLKP12, CAD16, HHWL17, JC16, KKK+17, KVQC+11, KLS10, KMLS10, KZP+18a, LZ12, LZX16, LZZ14, LZLMP16, MLIS10, MT19a, MBC11, MBC13, NST14, RSG+10, SLX+15, SDZ17, SJ17, SGY+18, SM15, SAvg15, WBF17]. **graining** [BJP15, GMPB12, ML14]. **Gram** [EVR18]. **Grand** [HLvdV13, PHH+12].

H [BSF18, BS16b, CXS10, CG12, CSNCS+18, DM15, DT19, GPK+16, HZ11, HSY+11, HVS16, JLS+10, JLH+14, LLL+11, LdSRR16, LAHS16, LWD13, MLQ+12, MCAY15, NMLD13, OKY18, OPR16, PMG+16, RMPAM15, Sak18, SNDK16, STS+10, TNY18, Tak11, TSJ+10, TFIG+11, UT14, UT15, VIT+15, VV14, WKC10a, WKLC12, WHT+10, WWS16, WLF19, WCL+11, XFX+16,
XCLZ19, YKH15, YZ15b, YZZ+17, ZYLL12, AS15a, Ben17, BS10b, CK10, CKL+11, Chu10, DT19, DHE+12, EVR18, GTK10, GS11, HZ11, HRL11, KTT16, LJW+17b, LWD13, MSPC19, Niz13, OKIS17, PLFS18, PTK11, Pie14, Pon10, STS+10, TS15a, TKCN19, UT15, UvSvdWK19, WGL12, WWTL19, WvRSM14, XhD15, XCLZ19, YHX19, YZ15b, YZZ+17, YZLZ18.

heterodimer [YYT12]. Heterogeneous
[DSF17, AFPI13, CKKK16, MEH18, RNS19, TM18, YZZ+17].
heterojunctions [FZL+19]. Heuristic [Hel13, MS16, Tak10, Tak18].
Heusler [GD10]. HeX [SLIB12]. hexa [GK15a]. hexa-aqua [GK15a].
heaxazatrinaphthylene [AWF+18]. heaxazatrinaphthylene-based
[AWF+18]. hexabenzocoronene [RVB+12]. hexacoordinated [MC10].
Hexahalogenated [VVJ15]. hexameric [RCM+13a, RML+15].
hexasilabenzen [NK19]. hexopyranose [HH11, PLH16].
hexopyranose-based [HH11, PLH16]. hexuple [XTn18]. HF
[BRLS12, LGW12, MCK17a, WZH+18, YZLZ19, BRLS08, Chu10, LSH+11,
SKGB13, YXH19, JT18]. HF-based [YZLZ19]. HF/DF [Chu10].
HF/DFT [BRLS12, BRLS08]. HFC [AR10]. HFC-263fb [AR10].
Hg [SLIB12, BBI+11]. HgGeCl [MCLD10]. HgHe [BBI+11]. HgXe [BBI+11].
HH [LGW12]. HI [LGW12]. hidden [DVVP14, LTT16]. Hierarchical
[JYC+16, BCG10, GBFD12, KKNN11, RMPAMP, SNS13]. High
[KLZ+18, MCLD10, MBK+13, RSLS13, ZHS+18, BACSCJ+10, Cam15,
CM13b, CSSB11, DH17, DLSL13, ESBL13, EKWK+13, FBvdB18, GJK+19,
GWPJ11, IPAA11, JBAM11, JC16, KSM16, KSM17, LL10a, LCK+18,
MJLV14a, MO17, OHPRL18, OPB+12, PV+13, PVJ10, RVCFF13, RNS19,
REH13, SML19, SC15, VWL+11, WDLG12, ZWL13, dSAdSL13, SDIP18].
high-accuracy [RVCFF13, SDIP18]. high-confidence [KSM17].
high-dimensional [FBvdB18, SML19]. High-level
[MCLD10, EKWK+13, KSM16, KSM17, PV+13]. high-order [REH13].
High-performance [RSLS13, CSSB11, ESBL13, EKWK+13, LL10a].
high-precision [DH17]. high-pressure [WDLG12]. High-quality
[MBK+13]. high-resolution [CM13b, JC16]. high-temperature [DLSL13].
high-throughput [ESBL13, PVJ10, RNS19]. higher
[NYH+17, PJ13, VKAM12, WHM10]. higher-dimensional [PJ13].
higher-order [NYH+17, VKAM12]. Highlighting [BRGN12]. Highly
[CHG+16, DBDP16, HAL14, LLZA12, LWP+16, BWK10a, BWK10b,
HYUS11, KOY+12, KZK+12, KV15b, OK16, TFQ+10, TBJ12, LZZ14].
hindrance [MP17a]. Hirshfeld
[Man13, VB13, VG+11, EV14, GBVA11, OVPK15, VB13a].
Hirshfeld-based [OVPK15]. Hirshfeld-I
[Man13, VB13, VG+11, VB13a]. histidine [KFY+13, WC14].
histogram [Fer17, HHWL17, SH11b, ZH12]. histone
[GHK12, GH10, GSD10, KCC1a]. HIV
[DLZ15, NHN16, OBW12, SYH12, TTB+10, UNT16, XLY12, Zsa10]. HIV-1
[DLZ15, NHN16, SYH12, TTB+10, UNT16, XLY12]. HIVgp41
HOB [LCL+10]. Hot [NMH19]. hole [BSF18, Cas13, CWHH11, EPH+13,
GZM16, GA12, LZL+15b, APK17, PTB+15]. holes [PM18a]. Holliday
[Ish10, She12]. hollow [AMAR18]. holographic [CDB10]. HotT [She12].

[AC12, HAGK10, RNS19, XTY+14, LHO17, LLJ12, She12]. identity
[Höf14, KN17, YN15]. IE [MLCD11]. IEF [GMMH+16]. IEF/PCM
[GMMH+16]. IEF/PCM-MST [GMMH+16]. Ihlenfeldt [PGPSM12]. II
[AMK11, ALH+10, BSG+18a, CMD13, CK17, FPB12, FB14b, GEP+14,
HRJ+14, HRJ+15, JIAB16, KPL15, LGW12, LWXC16, MLG18, MMB+17,
PHC13, SB10, TLA10, WGN+16, XP13, XWSW13, ZCK+16, vSGP10,
AKMYB18, BWKW10b, BB11c, CB11c, FXC+13, Fer13a, FVB10, HPT17,
HRJ+14, HWLW11, HHWL17, KTT16, KT12, KTNN10, KMLS10, MBC11,
PPUBGD10, SOD+11, WH11, YK13, ZSYH12]. III
[BP18, DSHLM18, IKN13, KPL15, LWL+11, LXZ+10, SRL+15, BGL+11,
CWT+12, GZZM16, HIS17, Zha12b, ZKH+10]. III/II [KPL15]. IKP
[HLS12]. Illuminating [NSO+14]. illustrating [RML+15]. illustration
[RP15]. im [FHC+19]. Image [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e,
Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n,
Ano12o, Ano12p, Ano12q, Ano12r, Ano12s, Ano12t, Ano13a, Ano13b, Ano13c,
Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13k, Ano13m,
Ano13n, Ano13o, Ano13p, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v,
Ano13w, Ano13x, Ano13y, Ano13z, Ano14a, Ano14b, Ano14c, Ano14d,
Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l,
Ano14m, Ano14n, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14t,
Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14-28, Ano14-29, Ano14-30,
Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14-35, Ano14-36, Ano14-37,
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Ano14-80, Ano14-81, Ano14-82, Ano14-83, Ano14-84, Ano14-85, Ano14-86,
Ano14-87, Ano14-88, Ano14-89, Ano14-90, Ano14-91, Ano14-92, Ano14-93,
Ano14-94, Ano14-95, Ano14-96, Ano14-97, Ano14-98, Ano14-99, Ano14-100,
Ano14-101, Ano14-102, Ano14-103, Ano14-104, Ano14-105, Ano14-106,
Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16c, Ano16s]. Image
[Ano16t, Ano16-37, Ano16-39, Ano16-42, Ano16-43, Ano16-44, Ano16-45,
Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52,
Ano16-53, Ano16-54, Ano16-55, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h,
Ano17a, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17z, Ano17-27,
Ano17-28, Ano17a, Ano17y, Ano17-29, Ano17-30, Ano17-31, Ano17-32,
Ano17-33, Ano17-34, Ano17b, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g,
Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17m, Ano17n, Ano17o,
Ano17p, Ano17q, Ano17r, Ano17s, Ano17a, Ano17t, Ano17u, Ano17v,
Ano18x, Ano18y, Ano18z, Ano18-27, Ano18-28, Ano18-30, Ano18-31,
Ano18-32, Ano18b, Ano18c, Ano18-29, Ano18-33, Ano18-34, Ano18-35,
Ano18-36, Ano18-37, Ano18-38, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g].

Image [Ano18h, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n,
Ano18o, Ano18p, Ano18q, Ano18r, Ano18s, Ano19a, Ano19f, Ano19g,
Ano19h, Ano19i, Ano19j, Ano19k, Ano19l, Ano19m, Ano19b, Ano19c,
Ano19d, Ano19e, Cor17, LCM16, SFLG+17, YHH+13]. images [LLJ12, MBFP15].
imaging [SCF+19]. imatinib [AS10]. imidazo [FD16, LWGZ15, NS10, YKH+10]. imidazolinone [CSC+18]. Imidazolium
[MG15]. imidogen [Kop15a]. Imine [DK19, AS11, GG10, HDB15]. imino
[GRCL12, YMY+19]. immediate [HTS17]. immersive [SFM+18]. Impact
[ABM+15, DPNM11, MCS11, MKK+19, VCL18, vADC+14, JMLL13, NW17].
impacts [SSNT19]. Implementation
[AMGB10, BMR11, HKR+14, HLEM18, ITIN15, KB14b, KK17b, LRvdSM15,
LPLA13, LBB+15, MHT+18, RJPB12, RSG14, SN16a, ZMMMI2, AB16a,
Boz18, BTB+11, CHG+16, Cas13, CEB015, CSSB11, EKW+13, KS13a,
KNHN16, KMLS10, KWG15, LL10a, LLZA12, LMR14, MKGA10, MBR+15,
MY+14, NYH+17, NLL19, NN18, OYK+11, QSY19, RSR+12, REV+17,
SSP19, SZX13a, SZX13b, TKT11, WPM+15]. implementations [LSD+10].
implemented [BVHI17, DLSA14, SR10, VBV13b]. Implementing
[Nav18, SCOJ13]. Implications
[CV12, VVY17, CBG16, LP11b, LTP11, RB12]. Implicit [BEM14, CAD16,
Has14, ALRM18, CBG16, EK15, FBEM11, KJDB12, KB11a, KB11b, LC17b,
ML14, SSBW14, SLX+15, SCMA+17, TCC+13, WWKS11, YL13]. implicit-solvent [WWKS11]. Importance
[APA+14, CPK12, ENKK+17, NFM+14, OOK11, ESM+12, Han11,
KTNN10, PBDW11, SDZ17, TNSS17, TKNN10]. important [AST+16, BZH14, MG11]. importing [FN12]. impregnated [GLZ17].
improve [CIKT13, DLL+10, DPSL16, Gou12, LLL+10, Min18, VLB+10].
Improved [BS16a, LRER13, CCM15, DPB+12, DSF17, GCCM15, KSR+16,
MP11, OHFR18, RTP+13, RDRC16, SSBW14, VVW+18, YS10].
improvement [GSHM10, NLP+16]. Improvements
[JCX10, AB16b, LRBB12, BB11c]. improves [BBOB16]. Improving
[AIM+18, DWL11, GS16, LN15, PLH16, RVM19, SB14, SACdG14, SA11,
Ano17-59, Ano17-60, Ano18-39, Ano18-66, Ano18-67, Ano18-68, Ano18-69, Ano18-40, Ano18-41, Ano18-42, Ano18-43, Ano18-44, Ano18-45, Ano18-46, Ano18-47, Ano18-48, Ano18-49, Ano18-50, Ano18-51, Ano18-52, Ano18-53, Ano18-54, Ano18-55, Ano18-56, Ano18-57, Ano18-58, Ano18-59, Ano18-60, Ano18-61, Ano18-62, Ano18-63, Ano18-64, Ano19n, Ano19o, Ano19q, Ano19r, Ano19s, Ano19t, Ano19u, Ano19v, Ano19w, Ano19x, Ano19y, Ano19z, BMPML\textsuperscript{+13}, CRZ\textsuperscript{+18}, CDS\textsuperscript{16}, CCYL\textsuperscript{11}, DWL\textsuperscript{11}, GBVA\textsuperscript{11}, ISN\textsuperscript{13}, RSL\textsuperscript{16}, ZLW\textsuperscript{10}. information-theoretic [CRZ\textsuperscript{+18}, ZLW\textsuperscript{10}]. informed [LZL\textsuperscript{+13}]. Infrared [EB18, DPA\textsuperscript{16}, HRR\textsuperscript{+17}, KB16, LBC\textsuperscript{+12}, NHF\textsuperscript{+10}, NPG\textsuperscript{+18}]. ingredients [CMvG\textsuperscript{10}]. Inherent [LLFH\textsuperscript{16}, Rao\textsuperscript{11}]. inhibition [BM\textsuperscript{12}, GWZ\textsuperscript{15}, LD\textsuperscript{18}, SSP\textsuperscript{+13}]. inhibitor [ETLS\textsuperscript{17}, FMG\textsuperscript{12}, LIL\textsuperscript{+11}, NFG\textsuperscript{+13}, XLY\textsuperscript{12}]. inhibitors [AKMT\textsuperscript{11}, ALW\textsuperscript{+10}, AC\textsuperscript{11a}, BM\textsuperscript{12}, DXY\textsuperscript{10}, DSX\textsuperscript{+11}, MPNS\textsuperscript{13}, NS\textsuperscript{10}, PBL\textsuperscript{dS\textsuperscript{12}}, RZG\textsuperscript{+13}, RAR\textsuperscript{+11}, SOD\textsuperscript{+11}, SJ\textsuperscript{16}, TTB\textsuperscript{+10}, VLB\textsuperscript{+10}, XDL\textsuperscript{+10}, YLCX\textsuperscript{10}]. Initial [GA\textsuperscript{18}, YLS\textsuperscript{19}]. initial-value [YLS\textsuperscript{19}]. initialization [GR\textsuperscript{11}]. initiate [HTS\textsuperscript{17}]. Initio [DHOG\textsuperscript{13}, Kop\textsuperscript{15b}, MSPC\textsuperscript{19}, PAK\textsuperscript{15}, RSR\textsuperscript{+12}, AR\textsuperscript{10}, AG\textsuperscript{12}, BEM\textsuperscript{14}, BLG\textsuperscript{10}, BIL\textsuperscript{+10}, DD\textsuperscript{S\textsuperscript{13}}, BL\textsuperscript{12}, CPR\textsuperscript{S\textsuperscript{18}}, CG\textsuperscript{15}, CLC\textsuperscript{11}, DCOD\textsuperscript{13}, DHF\textsuperscript{+11}, DLS\textsuperscript{13}, DJ\textsuperscript{13}, EP\textsuperscript{12}, EFO\textsuperscript{D\textsuperscript{13}}, FAA\textsuperscript{15}, FCD\textsuperscript{10}, GK\textsuperscript{10}, GZZ\textsuperscript{12}, HYD\textsuperscript{10}, KT\textsuperscript{19}, KOP\textsuperscript{+14}, KCC\textsuperscript{+18}, KTO\textsuperscript{11}, Kop\textsuperscript{15a}, Kop\textsuperscript{16}, Kop\textsuperscript{17a}, Kop\textsuperscript{18}, KSR\textsuperscript{+16}, Kow\textsuperscript{11}, KVR\textsuperscript{10}, LHL\textsuperscript{14}, LLP\textsuperscript{13}, LS\textsuperscript{10}, PBL\textsuperscript{dS\textsuperscript{12}}, RZG\textsuperscript{+13}, RAR\textsuperscript{+11}, SOD\textsuperscript{+11}, SJ\textsuperscript{16}, TTB\textsuperscript{+10}, VLB\textsuperscript{+10}, XDL\textsuperscript{+10}, YLCX\textsuperscript{10}]. inspection [KOY\textsuperscript{+12}]. inspired [CYY\textsuperscript{+17}, DSM\textsuperscript{+11}]. instability [MMH\textsuperscript{19}]. instantaneous [RO\textsuperscript{14a}]. Instanton [MK\textsuperscript{17}, MK\textsuperscript{19}, MR\textsuperscript{K\textsuperscript{11}}]. Insulator [GCC\textsuperscript{14}]. Insulin [MV\textsuperscript{17}]. INT [YJX\textsuperscript{13}]. INT-DBD [YJX\textsuperscript{13}]. integral [DL\textsuperscript{19}, KS\textsuperscript{NT\textsuperscript{19}}, MEH\textsuperscript{18}, RFN\textsuperscript{15}, SS\textsuperscript{13b}, Sn\textsuperscript{15}, VAT\textsuperscript{12}, WXY\textsuperscript{14}, YS\textsuperscript{18}]. integrals [CHC\textsuperscript{+13}, PS\textsuperscript{17}, PC\textsuperscript{16}, RLA\textsuperscript{18}, SZTS\textsuperscript{10}, WDKT\textsuperscript{19}]. integrase
Integrated [HSW⁺19, vRWGS17, CKKK16, MCC12, US11]. Integrating [APK14, LZZ14]. Integration [FPV13, AYYO17, BB11b, DH17, LP11a, MOS12, NSK18, dRL11, Pop13, Pop18, SJC11, SJ16, dRBO13, MYKO18]. integrator [JS17b]. intelligence [Aou16]. intelligent [CDS16]. Inter [CROB16, SSB11, IHY15, SSB13]. Inter- [CROB16, SSB11, SSB13]. inter-residue [IHY15]. Interacting [CM16, ATP18, EV14, HGCCGR⁺16, MP17a, PNE18, WL14, JCHT18]. Interaction [CK10, CCCLCGRO14, CCCLRO14, Den12, NNS15, SBW12, YZWC11, ALW⁺10, AG12, BLFZ13, BLF14, BCNH⁺11, BSD18, BHB⁺17, BRLS08, BRLS12, BG17, CLFR018, Cas13, CZHI2, CYG⁺15, CTP13, CAP17, EK17, EV14, FF11, FCCP17, FA18, GA14, GP11a, HPT17, HBL12, HLH⁺12, HSZ⁺11, HLXH17, HLXH18, HQSZ19, HL19, JZZM14, KAN15, KTN10, LL10a, LMZ11a, LPS⁺13, Li14a, LPHW14, LZL⁺15b, LPLB16, LWW11, Min18, MSĀK12, MCP18, MvBD18, NGAS17, NN18, OHP17, OHPR18, OAN15b, PRJ⁺17, RZG⁺13, RS13, SM16a, SS13a, SBBP18, SVB10, SGL⁺18, SPL⁺18, SHF11, TYN15, Tan19, TSH⁺19, WSH10, WYL⁺15, YK13, YWJ⁺16, YAO18, YCK16, YHCS11, ZRCC11, ZY14, ZW18, ZZI⁺19, dLvNC18b, vS18, KCB⁺12]. interaction-activation [LSL⁺19]. interaction-based [ZW18]. interaction-induced [BLFZ13]. Interactions [Sch18, WCT⁺11, ZCK⁺16, Abr11, ARR15, AKK⁺16, AO10, BSF18, BSG18a, CSS17, CC11b, CIKT13, cCVG⁺14, CKP10, CROB16, CB11a, CB1c, dRCFGRB18, DDP⁺18, DHF⁺11, DBG11, DLMH12, EP10, ER18, GWF11, GZZM16, GZ14, HSJ18, HLvdV13, HTY19, ICS⁺12, ICS⁺13, IHY15, JAB18a, KSSH13, KCK⁺15, KPH⁺19, KGJ19, LZLC13, LZY12b, MBGB16, MH17, MKH⁺13, MFR17, MJM⁺15, MVKS10, MG14, MFR⁺17, MPBJ11, OHNK11, PPJ14, PLV⁺11, RTS⁺13, RVM19, RMRH⁺19, SSGS15, SD12, SSB11, SSB13, TNSS17, TG12a, TY10, TGR⁺16, TNG⁺10, VVJ15, WS10, WGD⁺16, WDS⁺19, WZ19, WM17, XTY⁺14, XLY12, YKO⁺11, YZ15a, YW13, YZL⁺15, YGZ15, YZL18, ZZL⁺12, ZH11, dLC17, dLvNC18b]. Interactive [BRP⁺12, BGR13]. interactivity [CQFC10]. interatomic [DPABI, FCCP17, RLA18, YKO⁺11, dLC17]. interconversion [HH10]. interconversions [TCGT18]. Interdependence [WAB17]. interest [BCNH⁺11, OZLSBH12]. interface [All11, BDTP11, CSSB11, GRP⁺12, GC14, HL14, JJW⁺14, KG13, LIR⁺12, LZDL⁺10, LBB⁺15, MSSP17, NS18, OFYK⁺11, PHH⁺12, PVZ13, RTR14, RSR⁺12, SN16a, SYDS11, SISK10, STH⁺10, VKTRJ15, VL17b, WPM⁺15, ZWL13, SJL18]. interfaces [BB⁺18a, PGCT⁺12, RRF11, SSAS10]. interfacial [HTY19, NFDP13, SHFJ18]. Interfacing [MSvG12]. interference [KIOY19]. Interferometry [JAH⁺17]. interior [HL19]. intermediate [TDP⁺12]. intermediates [BL10, MRC⁺18, RB12]. Intermolecular [FMNC11, VECT12, ANO10a, BLF14, BLDK⁺13, CCLP12, KSNT19, KCL⁺14, LZY12b, LZLC13, RR12, SN10, TY10, TNG⁺10, VV12].
Internal [LL15, REH13, LWK+14, NCV10, PH10a, TNG+10, VLGGK+17, VBV13b, WBN+13, ALQ19].


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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, BG13, CTR13, DK19, GBGR16, HSB+ 19, HS16b,
KPL13, KPL15, MC10, NH19, SBC+ 11, TS10b, VBMA13, EH13].
iron-containing [AKMYB18]. iron-sulfur [CTR13, HSB+ 19, HS16b].
[TLY+ 12]. isoindolin [YZLZ18]. isoindolin- [YZLZ18]. Isolated [FL15].
Isomeric [FL15]. isomerism [RS17b]. Isomerization
[BW11b, DBGO+ 17, EFB16, BLG10, BMFG16, LL19, MSBF16, OKIS17,
SJD11, Su10, WCL+ 11, ZWZ11]. Isomers
[CSM16, ZWZ11, DSHLM18, Kar17, OKIS17, WCL+ 11]. Isoster [EdOdS18].
Isothiirane [MM19]. isotope
[KTT16, MRK11, NASH15, ORZ11, UT14, UT15, VKAM12, WXY14].
isotope-substituted [UT14]. isotopomers [UT14]. isotropic
[JKS+ 16, Tak14]. isotropy [Tru18]. Issue
[Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h,
Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano12o, Ano12p,
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Ano13y, Ano13l, Ano13w, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30,
Ano13-31, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h,
Ano13i, Ano13j, Ano13k, Ano13m, Ano13n, Ano13o, Ano13p, Ano13q,
Ano13r, Ano13s, Ano13-32, Ano13-51, Ano13-52, Ano13-53, Ano13-55,
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Ano14-32, Ano14-33, Ano14-34, Ano14c, Ano14z, Ano14-27, Ano14-48,
Ano14-49, Ano14-56, Ano14-57, Ano14-58, Ano14-59, Ano14-60, Ano14-61,
Ano14-62, Ano14-63, Ano14-64, Ano14-65, Ano14-66, Ano14-67, Ano14-68,
Ano14-69, Ano14-70, Ano14-71, Ano14-72, Ano14d, Ano14e, Ano14f, Ano15a,
[Ano15k, Ano15l, Ano15m, Ano15n, Ano15o, Ano15p, Ano15q, Ano15r,
Ano15s, Ano15t, Ano15u, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29,


iteration [SBB10]. Iterative [Hei18, VV19, Gra15, HLXH17, HLXH18, HL19, SM18, TTo19, VHR16, ZVY+15, PGL+15]. IV [EH13, KMS+19, MLG16, MTS+19, VBMA13, WZH+18]. iVI [HLXH18, HLXH17, HL19]. iVI-TD-DFT [HL19].


SHL +11]. **ligand-based** [RVP +11]. **ligand-binding**
[GDV17, MGWR12, OSR16, RO14b]. **ligand-field** [BBG +18b].
**ligand-induced** [KL14]. **ligand-receptor** [FRL10, VKC10]. **ligand-sized**
[OGL10]. **ligands** [CS17, GpDC +16, HRC13, KSO +19, LBC +19, LL10b,
LXZ +10, LS11b, SSP +13, TS10b, ZRCC12, ZWY +10b]. **ligated**
[EHI13, WC14]. **ligating** [BAD +19]. **LigDockCSA** [SHL +11]. **light**
[FWS +18, GNI18, HXM +16, KDR +18, PE11, REL17, XBSS19]. **light-driven**
[HXM +16, REL17]. **light-emitting** [FWS +18]. **light-harvesting**
[KDR +18]. **lighter** [WD10]. **Lightweight** [RLG14]. **like**
[AASP18, Che17, EPH +15, KOY +12, KD18, KB14b, MP17b, OAN15b, SDF +17, SM15, UCFR16,
VHA +10, VV18, WZF +18, WKC11, WGN +16, ZSL +11, VVY18, YLZ +19]. **Limit**
[SN16b, Fra15, Fra16, LW16, LYC +13, OAN15a, SLT14, WTH +16]. **Limitations**
[LVG13a, HH18]. **limiting** [SLT +15]. **limits** [GC18, II18, NSK18, PdSC18].
**line** [dLvNC18b]. **Linear** [BG12, NNT +19, XKW18, YN15, ZLY +16, ARLP13, CPY +12, EP12, FBY +17, FCE15, GZ12,
JJZ14, JMS13, KHM19, LP11b, MA17, MSÅK12, NYH +17, PH17, RS17a,
RLA +11, RR11, SS16a, Tak14, VBDS +11, WL10, YDX16, ZZ19].
**linear-combination-based** [Tak14]. **Linear-scaling**
[BG12, YN15, NYH +17, RR11]. **Linearity** [IKN13]. **linearized**
[Fra15, Fra16, XTn18]. **Ling** [Ano12u]. **Ling-Yun** [Ano12u]. **link**
[HH15]. **linkage** [HH11, OZS +13]. **linked** [Fom11, dACP12, LCC18]. **linked-cell**
[Fom11]. **linked-lists** [dACP12]. **linker** [NPG17]. **lipid**
[BPP17, MOS12, PGCT +12, ST11, WHAS +10, WHAS +16]. **lipids**
[HM16, ML14]. **lipopolysaccharide** [DLSA14]. **lipopolysaccharides**
[HB +17]. **Liquid** [WLC12, AASP18, APY +16, BDTP11, CC12a, EK15,
GWJR18, IM17, KGHC15, KT18, Lar12, MG15, NTTY15, RJS17, SBvG14,
SAvG15, WCWV15, ZST14]. **liquid/lithium** [EK15]. **liquids**
[AFP13, CG15, CFC15, CVG14, DASA15, LEDOLdV17, SCM +15, SH11,
You10, FDCJG18]. **lists** [Gon12, dACP12]. **liothiated** [KZK +12]. **lithium**
[EK15, GMG +10, KOY +14, KYCL11, LLY +11, MBRC16, NDI14, NIF +16,
PG12, PMT16, SKY +11, TN12, ZZ +12]. **lithium-bonded** [ZZ +12].
**lithium-doped** [PG12]. **lives** [QS19]. **load** [Fom11]. **LOBSTER**
[MDTD16]. **Local**
[CHP11, GH16a, GH16b, HKJ13, ITIN15, CPN +17, DDP16, Fer13a, HH10,
KSSH13, KDT +12, KGM12, Lar12, LLL +10, LZS +17, MKH +13, NLL19, PH17,
PRSG13, PRY +17, PW12, Ran19, RVM19, Sch12, SEF +16, SB15, WM17].
**locality** [Gon12]. **localizability** [Bar14, BLG11, BKWK10a, BKWK10b].
**Localization** [Sax12, ABG11, BK11, BLG11, GNDA +12, HJJ13, Mat14,
Pil17, dLC18a, vSGP10]. **localized**
[Ano15-58, BH14, KKH18, SB15, ZM11, dLC17]. **locate** [AMGB10].
**location** [PTB +15]. **locked** [GA18, XVN17]. **locking** [XVN17]. **locus**
[NR11]. **logarithmic** [MIOM13]. **LOL** [BSPP +13]. **lone**
[BSF18, BS18a, ENS17, SSGS15, WCY +11]. **lone-pairs** [ENKK +17].
**Long** [BCNH +11, KSH13, KSSH13, AO10, BLBG +13, BZH14, JBSQG11,
KB10, KV14, MMS16, MBC13, PNG10, SMGB11, ST13, SPH11, SH19, SZB19, SSA17, TSN16, VL17a, VCL18, Rui11. long-bond [KV14].

long-chain [TSN16]. Long-range [BCNH11, KSH13, KSSH13, KB10, MMS16, ST13, SPH11, SH19, SZB19, SSA17, VCL18, Rui11].


Low [BPM15, BLDK13, Gra15, AC12, CM13a, DH14, KKA18, LG14, MPA10, MPA12, MJLV14a, RRC15, SN15, SG10a, SM11, She12, TF15, TSN17, UGK18, Vor10, YW12, BS10c, BBI11, SGP18].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

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Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].

Low-energy [BPM15, DH14, MPA10, MPA12, SGP18]. low-index [RRC15]. low-lying [AC12, KKA18, TSN17]. Low-memory [Gra15].
Many-body [CGPP11, HRJ+14, HRJ+15, JRSHP14, LYC+13, RHPWS13, VMPS17].

many-core [KNHN16], map [MKM+17], mapper [BJP15], mapping [EMD17, KZP+18b, MMM+16, RNRF+16, TD10]. maps [GJMPPAM+14, YSRS10].

Marburg [OLY17]. marker [JAH+17]. Markov [BFH+13, LTT16].

Martini [HBJ+17, SM15, MT19a]. MARTINI-like [SM15]. mass [NPTS16, PGY15]. massive [GP11b, TNYN16].

Massively [KNHN16, KZZ+16, KN17, NNK+16, OPB+12, WHK+12, KCC+18]. master [RSLS13, NNT+19]. match [TZ12, YPKB12]. matched [KSR+16]. matching [AOW11, GPS10, HS12].

Material [JW12, DGL+13, HLWD15, JBSQG11, LL13b, MCAG+16, NGAS17, SHL19, SMiN+19, SLHW09]. materials [BSL+16, CD11, DLT17, ECZWD17, EMD17, GNI18, KLZ+18, Man13, NDD+10, SB18, SYZ+17, VBV13a, VBV13, VVY17, VVMM18, YZLZ19].

MATLAB [DDK14]. matrices [Car14, LHO17, Mat14, Yon16]. matrix [CAP17, CWZB10, Kne11b, LAT10, LAT11, PW12, RPNP10, RNP13, RR11, SS13a, STM17, TCPPC14, UIW+10, VGV+11, VKNT15, VKNT16, ZVY+15].

matrix-based [VGV+11]. matrix-free [ZVY+15].

[HLH_{12}, KSK_{11}]. methylacetylene [WCWW_{11}]. methylated [LRVM_{18}]. Methylation [SCW_{11}, KYCL_{11}, QZM_{11}, dALdS_{15}]. methylbenzyl [NDG_{14}]. methylcobalamin [KKL_{13}]. methylformamides [JSW_{10}]. methyllysine [GHK_{12}]. methyltransferase [CPLL_{11}, GH10, PBLdS_{12}]. Methyluracil [HvM_{17}, HvM_{16}]. MetREx [Sti_{15}]. metric [CXS_{10}, LLFH_{16}, PKIC_{11}, SOJ_{14}, ZT_{14}]. metrics [Hug_{14}, PBBP_{11}, RCM_{13}]. Metropolis [MO_{15}, Pon_{10}]. Mezey [HJJ_{13}]. MF [YKH_{15}]. Mg [LDJ_{10}, LLX_{19}, BMFG_{16}, DOM_{11}, PLZ_{17}, PGY_{15}, RRF_{11}, SS13c, ZZ_{10}]. Mg-porphyrin-based [PLZ_{17}]. MgO [BS_{16}]. MH [HHT_{13a}, HHT_{13b}]. MHC [HHWL_{17}]. MIA-QSAR [BF_{15}]. MIBPB [CCC_{11}]. Micellar [SCK_{18}]. Michael [NDG_{14}]. microbes [RSLS_{13}]. microclusters [NC_{12}]. microelectrostatic [SMP_{17b}]. microhydration [SM_{17}, ZYR_{15}]. microiteration [SMM_{17}]. microscopic [HLWD_{15}]. microscopy [LLJ_{12}]. Microsecond [DMN_{14}]. microstructures [DASA_{15}]. microwave [BLF_{14}]. MIDAS [GJMPAM_{14}]. Midpoint [JMS_{14}]. migration [FBEM_{11}, Ish_{10}, KYKR_{15}, RSB_{13}, TN_{10}]. milestoneing [BRE_{16}]. mimetic [MV_{17}]. mimetics [CFM_{19}]. mimic [GRP_{12}, ZWS_{10}]. mineral [TZ_{11}]. mini [CFC_{15}, HTS_{15}]. mini-protein [CFC_{15}, HTS_{15}]. mini-proteins [HTS_{17}]. minima [AC_{12}, GFG_{11}, HvMi_{12}, MAMF_{19}, SGWA_{17}]. minimal [CGBK_{13}, CG_{12}, OYK_{11}, RSR_{12}, RVVK_{13}, WHAS_{10}, WHAS_{16}]. minimization [GBV_{11}, Rao_{11}, TJB_{12}, XHLH_{16}]. minimized [ZA_{15}]. minimizing [KS_{12}]. Minimum [RAR_{11}, CY_{09}, CY_{13}, CZZL_{19}, HNYH_{19}, LLSW_{14}, MP_{13}, MCAY_{15}, PRP_{15}, PHDH_{13}, SRSLO_{15}, SG10b, Tak_{10}, MYKO_{18}]. mining [BCP_{10}, MCC_{12}]. miniprotein [MTD_{10}]. minnesota [LH_{14a}]. minnesota-type [LH_{14a}]. minnow [TTL_{12}]. misfolding [LH_{11}]. mismatched [BH_{13}]. mispair [BZH_{14}]. Mixed [RdA_{12}, BRGN_{12}, BEEL_{14}, BACSCJ_{10}, DH_{11}, DFF_{15}, Fer_{13b}, Fer_{13a}, GMASBF_{16}, GG_{10}, Ibr_{17}, JT_{18}, KGR_{16}, LYL_{16}, MP_{13}, PsdPE_{10}, RB_{12}, TS_{10b}, VVJ_{15}, WX_{12}, YLL_{11}, SZL_{19}]. mixed-basis [WX_{12}]. mixed-QSPR [BRGN_{12}]. mixed-resolution [DFF_{15}]. mixed-valence [BEEL_{14}, KGR_{16}, SZL_{19}]. mixing [LCH_{10}, ZA_{15}]. mixture [BBJ_{11}, MKB_{13}, RHN_{10}]. mixtures [GM_{17}, GC_{11}, JA_{10}, KGHC_{15}, SV_{11}, TKYN_{17}]. Mizoroki [dSdB_{17}]. MLR [GCP_{13}, XWW_{11}]. MM [BM_{12}, JAHS_{19}, LWZ_{19}, AALCM_{11}, BTA_{13}, BD_{11}, CZY_{11}, CS_{17}, CIZS_{10}, DSK_{17}, DSX_{11}, FLM_{11}, FPD_{12}, FB{14b}, GR10a, GRS_{15}, GWZ_{15}, GCW_{14}, HH_{15}, HBR_{17}, IMSR_{18}, JJJ_{13}, JWST_{10}, KTN_{10}, KWL_{16}, KWG_{15}, LZdL_{10}, LFM_{12}, LT_{13}, LHT_{15}, LJJ_{11}, MCRL_{17}, MTvG_{12}, MJG_{15}, NO_{16}, OBW_{12}, PMC_{17}, PDMT_{10}, PL_{14}, RDDS_{10}, RFN_{15}].
RR14, RN17, RR12, SN16a, SGDT10, SJD14, SCM+15, STM+15, SSAS10, TSC+13, VKNT15, VKNT16, VCM15, VKTRJ15, VM11, WDP+12, ZZY+16.

**MM-GBSA** [RDDS10]. **MM-MD** [RSR+12, OYK+11]. **MM-PB** [OBW12]. **MM-PBSA** [RDDS10]. **MM-QMC** [UTM11]. **MM/GBSA** [GR10a, IMSR18]. **MM/PB** [VM11]. **MM/PBSA** [BD11]. **MM2QM** [NHK+13]. **MMGBSA** [GS14]. **MMPBSA** [WNP+16]. **MMX** [CRC13].

**Mo** [BRP+12, UIW+10, ZY14]. **moana** [DJ12].

**mobilities** [SEF16]. **Mode** [AIM+18, BHR15, GVP+10, IY18, SRA17, SBB10, YHCS11, XYZZ17].

**Mode-tracking** [BHR15]. **Model** [BLS10, HM16, Pog10, AASP18, AOW11, AS10, ALRM18, ATP18, AS15b, APA+14, AB16b, Bac12, BK17a, BEEL14, BS10b, BBG+18b, Cam15, Can10, Can11, CGP12, CGA19, CBTZ16, CFC15, CAD16, CG12, CMS13, CJZS10, DLL+10, DSF17, FCE15, FNSF+11, GRS15, GM17, Gil11, GKR13, HLS12, HAL14, HLH+12, HOK17, HZSS17, Hug12, HRR+17, ISO+13, IN13, IL18, JSXH16, Jor17, KFY+13, KCK+17, KMS+19, KR12, KOY+12, K18, KCPMG12, KBI4b, KDS17, LSL+19, LTT16, LY10, LRvdSM15, LFN+10, LPS+13, LHWH14, LZZ+15a, LDG+15, LCK+18, LHMM11, MSL10, MT19a, MBC11, MBC13, MMB+17, MOH18, NIX+10, NTNY15, OPBR17, PB14, PCLI11, Pla11, Pon11, Ray13, RTS+13, Ric16, RMRBH+19, REL+14, RKG11, SM14b, SDF+17, SHF11, SSBW14, SK12, SK17, SLX+15, SDZ17, SZBM13, SB11, TYN15, TCC+13]. **model** [Tia12, TLA10, TTn19, UIW+10, VV14, VHS+19, WWKS11, WXL+12, WC13, WNM17, WRHF10, WKC11, WCAH10, XZ11, XTY+14, XP13, YS18, YOMT14, YB13, YSG12, ZST14, ZKH+10, ZM10, dSDDAR10, CCR18, FAS+18, MJBM12]. **model-tuned** [HZSS17]. **modeled** [MPA12]. **modeler** [KLJ+17]. **Modeling** [CB11a, DLSA14, FD13, FTW12, GMG+10, GBS+17, HPL13, JW16, KDR+18, Mat14, NS10, NDLW13, PLP+16, SK11, Tia12, Vyb15, AKMT11, Aou16, BEM14, BCP13, Bow16, BS10c, CMD13, CLA16, CZNA11, DAG19, DWR17, D5X+11, DLMH12, EBPK17a, FXC+13, GH10, GP12, GMZ12, GWJR18, GR10b, GWZX12, HLvdV13, HBJ+17, JC16, JCL+17, KSD+12, LABSG17, LHLH14, LZG11, LT13, LN15, MBA11, MJLV4b, MA17, MBA14, MPBJ11, NSO+14, NW17, PHC13, PSS14, PSS+17, PMT16, QLKI19, RJS17, SN16a, SKGP19, TTR+12, VKNT15, VAA14, VCM15, WXL17, WPM+15, WLO+17, XDL+10, XLY12, YMY+19, YJ11, ZX11, DHE+12].

**modelling** [DBM+15]. **models** [BEM14, BLKP12, BPB11, CD11, Cor17, CBG16, CK17, DDP16, DSM+11, DI11, DGC14, DCL18b, EK15, EPD+10, GMPB12, GMMH+16, GMG+10, GKR13, GCP+13, GCC14, GAJ+17, HS16b, HGY15, JCP14, JGS+17, KJDB12, KKO+16, KB11b, KSR+16, KSW16, LTT16, LKL10, LZZ12, LLSW14, LM18b, MPSA17, MSA12, MCU15, MKB+13, NNS15, OL13, PHC13, PGY15, PL18, Ray13, RTP+13, RKG11, SPHF+18, SCMA+17, SFLG+17, SAVG15, TH13, TTB+11, TTL+12, VKC10, VMPS17, VZ14,
modern [AB16a, AB16b, DH17, Fom11, LMR14, SF18, SDM +16]. modes [CBP +15, EB18, GMPB12, KKHH18, LLTC12, MS17, dSAdSL13].

modification [Ano12u, MIS +15]. modified [BD12, CH16, DPSL16, DJX +11b, GSD10, MRO17, Mit13, SMM15a, SMM15b, SMM +18, XXY17, XVA +16, ZZ12]. Modifying [CYG +15, LBS10].


MOFs [LPK16]. moieties [SPL +18]. MOLCAS [ADF +10, VBV13b, AAC +16].

Moldyn [HPSK12]. Molecular [AASP18, BDTP11, BSF18, CRZ +16, CBP14, CMM18, CCR18, CM13a, CDBM11, Car14, CTR13, CAF +13, CEBO15, CGA19, CIKT13, CGPP11, CS14, CXW14, CBTZ16, CH16, CCOH14, CVG14, CCW +10, CHKR10, CJPTC18, CB11b, CB11c].

molecular [CM16, DMJ17, DSD +11, DJX +11b, DJX +11a, DJS +18, DLZ15, DDM +15, DN19, DL19, DL16, EP10, EK15, EJ13, EPH +13, EPH +15, ENKK +17, EPD +11, Fer13b, Fer13a, FBvdB18, FBEM11, FSC +14, GBL +11, GDV17, Gar12, GJMT14, AG11, AST +16, APFI13, AS15a, ASL +11, AS10, APK14, AS18, AGB13, AS15b, AGR11b, AJR16, AB16a, ASK18, ALH +10, BMRI11, BAMR13, BEM14, BSL11, BF15, BBOB16, BJS12, BV14, BW15, BF17, BJP15, BGL +18, BMBJ11, BE16, BS18, BVC13, BEL +11, CBP14, CMM18, CCR18, CM13a, CDBM11, CD13, Car14, CTR13, CAF +13, CEBO15, CGA19, CIKT13, CGPP11, CS14, CXW14, CBTZ16, CH16, CCOH14, CVG14, CCW +10, CHKR10, CJPTC18, CB11b, CB11c].

molecular [CM16, DMJ17, DSD +11, DJX +11b, DJX +11a, DJS +18, DLZ15, DDM +15, DN19, DL19, DL16, EP10, EK15, EJ13, EPH +13, EPH +15, ENKK +17, EPD +11, Fer13b, Fer13a, FBvdB18, FBEM11, FSC +14, GBL +11, GDV17, Gar12, GJMT14, AG11, AST +16, APFI13, AS15a, ASL +11, AS10, APK14, AS18, AGB13, AS15b, AGR11b, AJR16, AB16a, ASK18, ALH +10, BMRI11, BAMR13, BEM14, BSL11, BF15, BBOB16, BJS12, BV14, BW15, BF17, BJP15, BGL +18, BMBJ11, BE16, BS18, BVC13, BEL +11, CBP14, CMM18, CCR18, CM13a, CDBM11, CD13, Car14, CTR13, CAF +13, CEBO15, CGA19, CIKT13, CGPP11, CS14, CXW14, CBTZ16, CH16, CCOH14, CVG14, CCW +10, CHKR10, CJPTC18, CB11b, CB11c].
OME16, OVPK15, OOT15, OCW+15, OZS+13, OOK11, PMC+17, PSS14, PAK15, PK17, PH17, PSG+17, PM13, PGW+17, PVZ13, PJ13, PGB17, PS10, PVAM16, PLP+16, Pro16, PH15, PVJ10, RJBH18, RD18, RMPAM15, RLLHL12, RN5F+16, RNPI3]. **molecular** [RNV13, RS12, Ras17, RHJ11, RO14b, RR14, RdA12, RC18, RLGI4, RSR15, REH13, SHMO19, SF18, SLT+15, Sax12, SWM10, SK15b, SA13, SZTSM10, Sch12, SFR+11, SHFJ18, SHF11, SMRM+17, SS19, SSNT19, SOM+13, SJ17, SR18, SYN+12, SK13, SWB+12, SLLL13, SJ16, SDMS13, SKY+11, SZZ+18, SPZP18a, SPZP19, SBV14, SAVG15, TNY16, TKN10, TZ12, TCT+18, US11, UGK18, VYMI5, Vik11, Vor10, Vor12, VM11, WKLC12, WBN+13, WAM17, WLW+10, WH11, WCY+11, WLC12, WOH16, WXL17, WOH18, WES13, WB17, WCDM11, WO15, WCV15, WL14, WGI4, Won18, WDKT19, XDL+10, XG+15, YKO+11, YPvD13, YNH+17, YLGX14, YLCX10, Yap11, YPKB12, Yes12, Yes15, Yon16, ZSTI14, ZWL13, ZZ+16, ZX11, ZDKM12, ZSS+13, ZLY+16, ZP13, ZWX16, ZLL+13, ZA15, ZBmZH15, dSLBNB17, dCLFL13, dLvNC18a, AIM+18]. **Molecular** [IPAA11, KSD+12, MJLV14b, ZBP11, ZKH+10]. **molecular-mechanical** [ZSTI14]. **molecular-orbital** [US11]. **Molecularnetworks** [MCC12]. **Molecule** [KR12, vRG17, BT18, DHOG13, DGL+13, ETL17, FAA15, GAI14, GCWS15, GBVA11, HLvdV13, HHH17, ISO+13, IIHY15, KB11b, KKA+18, LIRL+16, MCUJ15, NLL19, PC11, RLL+10, SG10b, VGV+11, WF16, XYW+14, XMS16]. **molecule-mediated** [XYW+14]. **Molecule-specific** [KR12]. **molecule-transcription** [XMS16]. **Molecules** [ATM18, PdSC18, AIG15, Ali18, AWF+18, ARAG17, AGR11a, BLBG+13, BS10a, BTMS12, BS18, Ben17, BS16b, BL12, CFZ19, CHG+16, CC18c, CQF10, CYG+15, COOH14, CXS10, CZNA11, FE14, GWF11, GJK+19, GP12, GPGM11, GPGM12, GAJ+17, HBR+17, HSB+11, Hug12, Ihi12, Kan15, KLJ+17, KJZ19, KYG+15, LPS12, LHS12, Lw13b, Lju14b, LjL+11, LG14, MA16, MS13, Mat10, MSS+13, MH17, MBE16, MPB11, NIT15, OGL10, OT12, PB13, Pyy13, RS18, RSG14, RK15, SFCCK+14, SFCCK15, Sch13, SG10b, SFLG+17, SY16b, SM17, TZK18, Tsr+16, UNT16, VVY+15a, VHA+10, VVY18, VDVR14, WC13, WSZW15, WWD14, WX12, You10, YK15, YHW17, ZPP+16, Zha12b, ZLX+13, ZBB16, ZGGM11, MSPC19, SMB18]. **Møller** [SSW17, Hii13, KKK11, KN17, MCC11, YKH15]. **MOLSIM** [JP15]. **molSimplify** [GK16]. **molten** [LCL+18]. **MolTPC** [WHJ13]. **molUP** [FRC18]. **Molybdatricarbaboranes** [LK16b]. **molybdenocine** [PM13, SDL14]. **Moment** [SS16a, JCG+11, KCB+12, Yan11]. **Moments** [GH16b, Ali18, BLDK+13, CP15, CTP13, DHOG13, GH16a, Lar11, NOK16, Tru18]. **momentum** [EP12, GWF11, NCT18, PH17]. **monazite** [RKB+14]. **monazite-type** [RKB+14]. **mono** [HV19]. **mono-** [HV19]. **monoaion** [YZGS14a]. **monoboronyl** [VVBL17]. **monohydroxide** [Kop17a]. **monolayered** [RSKG14]. **monolayers** [LD12, RSK+15]. **Monomer** [SC17]. **Monomeric** [LLT12, CAT+13]. **mononuclear** [BCSCJ+13, OSS10].
[AS15a, FTR15, JWO15, KHE+19, OCW+15, RHNN10]. **nanotubes** [ASL+11, BE14, BPE16, DI11, Den12, DZA11, EBK13, EP15, EBPK17a, EBPK17b, EB18, GBS+17, KGHK12, KGJZ19, LPLS16, LL10c, LT14, MSY19, NDD+10, PBE16, TD11, TSR+16, VS14, WYL+15, WDZN16, YZN13]. **nanowires** [EP15]. **naphthalenediimides** [MSG+16]. **naphtho** [ZLL+10]. **naphtho-homologated** [ZLL+10]. **naphthodithiophene** [DGL+13]. **naphthol** [CYY+17, GZL+12]. **naphthoquinone** [HWB19]. **naphthyl** [CFM+19]. **naphthyl-based** [CFM+19]. **NARES** [SGY+18]. **NARES-2P** [SGY+18]. **native** [DJ13, HYL+11, UCFR16, YL13]. **native-like** [UCFR16]. **Natural** [LCPS13, MBFP15, SZL19, Wei12a, Wei12b, AO10, GMZ12, NC14, Sch12, AIQ19, GLW13a, GLW13b, Spr18]. **naturally** [XVA+16]. **Nature** [ABDGN12, MJM+15, SC18a, WFZ+18, GPK+16, GA19, HBR17, Kri10, LZJ+11, LLY16, LdSRR16, LTR18, MLGB16, PKK17, RKDM14, YK13, YJ17, ZRCC12, dLvNC18b]. **navigation** [SLG15]. **NBe** [UT14]. **NBO** [GLW13a, GLW13b, WvRSM14]. **NBS** [YZ17]. **NCCH** [MLGB16]. **NCI** [REV+17, VVJ15]. **NCX** [LZL+15b]. **NCY** [LZL+15b]. **near** [DJ13, NPG+18, Yan11]. **near-infrared** [NPG+18]. **near-native** [DJ13]. **near-solute** [Yan11]. **nearly** [LPS12]. **necessarily** [Jab18a]. **Necessity** [JC16]. **necks** [CC12a]. **Negative** [PG18, KV13]. **neglect** [WDKT19]. **neighbor** [AGR11a]. **neighboring** [HSJ18]. **NEMO** [HBKL10]. **nesting** [HSB+19]. **Net** [RO14b, CS14]. **netropsin** [HDK+12]. **network** [AD10, GFPSD17, GGM+12, HNNR13, HAT+16, IHY15, JCY10, LDH+14, NSK18, OC14, FC11, PPUBGD10, RKDM14, SHL19, WMW+10, XTY+14]. **network-based** [PC11, PPUBGD10]. **networks** [AGM+13, Clo15, Kan15, KUDG12, LHO17, PPM15, PPUBGD10, TD11, WZWW18]. **neural** [AGM+13, HNNR13, LHO17, LDH+14, PC11, SHL19, WMW+10, WZWW18]. **neutral** [AM19, GC11, GWPJ11, JM11, KDD10, Tsi14, GMBM18]. **new-type** [HLWD15]. **News** [AIGP15, AKI16, APK14, AAC+16, GTA+13, BHH12, BCSCJ+13, BSZ+12, Ber17, BJP15, BFH+13, BBG+18b, CBH14, CSEMB+16, CZAF17, CAT+13, DMN15, DJD12, DVVP14, DBDP16, DDK14, DWC17, DSK17, ES13, EWE+13, FNI12, FSC+14, GMSdG15, Gar12, GJMPAM+14, GLW13b, GS12, GCP+13, GCC14, GBW+14, GH16b, HLS+13, HRB+17, HDH12, HPT+16b, HPS12, HHT+13b, HH16b, HG13, HMYM16, HKR+14, HBJ+17, HLC14, IGK16, JHH+13, JJJ+14, JLCA17, JP15, JCGM18, KS13a, KS15, KK17a, Kan15, KB16, KDR+18, KLJ+17, KJM+17, KDT+12, Kos16, KG13, KWL+16, KK17b, KGW15, KYG+15, KAG+12, KSW16, KPF+15, LPS12, LJ+12, LHS12, Leh15, LRvdSM15, LRvE17, LDB+17, LLZA12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MDT16, MBR+15, MYT18, MSSP17, MB14, MB16, NKJ16, OV14, OPB+12, OZS+13, OC14]. **News** [FSS14, PGL+15, PSG+17, PW12, PPM15, PHH+12, PVZ13, PG14, RLLHL12, RNSF+16, Ras17, Rex16, RR14, RdA12, RSR+12, KRM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sie15, SJ17, SWB+12,
Nitrogen

SDMS13, TNYN16, TSC+13, TTR+12, TTL+12, UU12, VMRS+17, VVV+15b, VAR12, VBV13b, WDVN12, WDY13, WPM+15, WF16, Wei12b, WHK+12, WHJH13, WGI4, WCJ+14, XML+15, XYX17, YWJ+16, YZZ16, Yes12, Yes15, YHH+13, ZDKM12, ZL+13, dVAG16, KKR+13. Next


[CG12, KSK11, LLX+19, LBT12, VVY17, CCJ+11, Kop15a, LYYC+13, LBTV11, ONTTL16, UT14, Yu12a]. NHC [GA19]. NHCHO [KMS+19].

[NH· · · [MVK10]. NHH [LZH+11]. NHOC [LHHW14]. Ni

[Ibr17, MP19a, TLDG+12, Tsi17, WWS16, ZFS18, MMB+17, SIT18, SSX+14, TLA10, ZRC12]. Ni-NO [Tsi17]. Nickel

[SMB18, ED15, FCW+14, HVS+19]. nicotine [PMC+17]. NICSz


[YPC+10, ZWZ11, FAS+18].

Nitro-Porphyrin [FAS+18]. nitro-substituted [YPC+10]. nitroaldol

[QLY10]. nitroaniline [ZTH+15]. nitroarenes [MRC+18]. nitroaromatic

[PSC11, SB18, TD10]. nitrobenzenes [ZGS+10]. nitrocompounds

[SIG+15, SGH+16]. nitrodibenzo furan [DPB+12]. nitroethane [YZL+15].

Nitrogen [LLC17, BEPM14, KV14, Lin18, ZZWX11, ZYL+12, SMD18].

nitrogen-atom [KV14]. Nitrogen-doped [LLC17, Lin18]. nitrogen-rich

[ZZWX11, ZYL+12]. nitrogen-substituted [BEM14]. nitrogenase [Sie18].

nitroiminotetrazolate [ZYL+12]. nitromethane [MCU15]. nitrosamine

dALdS+15]. nitroso [TDP+12]. nitrosothiol [TKXT13]. NMR

[Ben17, CHP11, EOA+11, HJ13, HBI+17, HM13, KASH14, LD11, ORP16, PTK11, PGdO+16, PC14, Pie14, RK15, SPHF+18, SEF+16, SKMS13, SPZP18b, SPZP19, TET18, WL14, YS13]. NNO [WGL+11]. NO

[MCU15, Tsi17, ZZ10, WYGW12, BS16a, GY12, LWZ+19, MN19, OSH17, RGCVC+19, TNI+19a]. Noble

[SMD18, ARLP13, GC18, JKS+16, PGS+15, PMG+16]. NOCV

[CSM16, DBGO+17]. node [KK17a]. nodes [KPF+15]. NOEs [LK11]. Non

[KB11c, LCH10, BSD18, CSKH15, GMZ12, GA19, HOK17, MR17, NHN16, PHC13, RS13, VCL18, YWJ+16]. Non-Boltzmann [KB11c]. non-bonded

[BS18]. Non-Born [LCH10]. non-classical [GA19]. non-covalent

[MR17, RS13]. non-electrostatic [HOK17]. non-empirically [VCL18].

non-equilibrium [NH16]. non-heme [PHC13]. non-hybrid [CSKH15].

non-natural [GM12]. non-uniform [YWJ+16]. nonadditive [RTS+13].

Nonadiabatic

[HZ11, RGYC+19, JBSQG11, KIOY19, MT19b, SRSLO15, WLF19].

nonadiabaticity [Wn10]. nonbonded [Abr11, EP10]. Noncatalytic

[SGS+16]. Nonclassical [GZH10, DM15]. Noncovalent

dRCFGRB18, Sch18, RRRH12, RLA18, SM16a, SBW12, TSR+16, VT14, WGD+16, WDS+19, YW13, YZLZ18, SMD18]. noncyclic [SM16a].

nonempirical [BK17b, WYT17]. nonequilibrium [ASL+11, KHWB17].
Nonfitting [RZG+13]. nongeometric [KB11a]. nonheme [BG13].
Nonlinear [LLX+19, ARLP13, KOP+14, LLd17, MLQ+12, MIS+15, RLA+11, TFQ+10, Tia12, YCGA10]. nonlinear-optical [KOP+14].
noniterative [RB13a]. nonperiodic [MS15]. nonplanar [KG11].
nonnorbornadiene [Ant13, WJX+10]. normal [GVP+10, GMPB12, KKH18, MS17, SBB10, IY18].
Notes [CD13]. Novel [FCL+10, KKO+16, RPNP10, AIGP15, BEPM14, BPM15, DFWL11, MDL14, RNP13, WKC11, YJN+11, YHCS11, YDGZ15].
novo [AFBR17, BAMR13, LK11, MDT10]. Nuclear [ASK18, DKT13, ECZWD17, KN+12, CSEMB+16, HH16a, HH17, JKS+16, MT19b, NASH15, PLFS18, RSG14, SPHF+18, SS13b]. Nuclear-step [ECZWD17].
Nucleic [HGY15, ZWP11, F10, FCE15, GREA11, MSL10, OX16, SCF+19, SGB+18, SBW12, WGL12, XV17, ZSB+11]. nucleic-acid [SGY+18].
nylon-oligomer [BHNS14].

O [AM19, BCNH+11, CXS10, CSNCS+18, DHE+12, GBGR16, HRL11, JM11, JLH+14, KMS+19, LZTV10, LLLM11, LLB+12, LSW14, MG11, PLFS18, PBE16, RHT+15, SPS+12, SBD+17, TNY18, VV14, WLL+10, WLF19, WRG+12, XFX+16, YW12, YR13, YOPB16, ZRCC12, Tsi17, BCNH+11, BWK10b, CK10, Chn10, HOB16, CPLL11, D19, DHE+12, HZ11, LZW+15b, LCWW10, MH11, MSC19, MS15, PBLdS12, RHN10, RAGL11, SZ17, SJD16, SXX+14, TKCN19, WLF19, Y15b, ZRCC11, ZSW12, dCRN18]. o-atom [Tsi17]. O-H [TKCN19]. O-loss [MH11].
Obtained [GR10a, GR11, MA16]. obtained [LRVM18, OSR16, SISK10, Tak10].
obtaining [STM17]. occlusion [BK17a]. occupancy [MP13]. occupied
[HJJ13, MRB14]. occupied-virtual [MRB14]. occurring [XVA+16]. ocean
[SSNT19]. OCF [ZLL12]. OCHO [dCRN18]. octa [ABDGN12, CC18b].
octa-1 [ABDGN12]. Octene [MJLV14a]. OCXR [FCOGM12]. OD [Chu10].
off [RGVC+19, WZ19]. off-diagonal [WZ19]. offsets [KRSC12]. OFLOW
[HNS16, HNTS15]. OH [CXW14, Chu10, GTK10, HZ11, LLSW14, AR10,
CK10, CSNCS+18, GK10, LJW+11b, LJG+11, RAGLL11, SST+18, TSJ+10,
VDRV14, WLHZ12, ZZL+10a]. OH/OD [Chu10]. OH ··· [MVKS10].
OHHGe [WHX+10]. oils [ZSTI14]. Ole [Spr10]. olefin
[KSO+19, MJLV14b, RS17b, MTS+19]. olefins [BF19]. olfactory [DR14].
oligo [KSW16, TZ12]. oligo- [KSW16]. oligoacene [HZSS17]. oligomer
[BHNS14]. oligomerization [KAR12, ZQ14]. oligomers
[DP15, PH10b, ZSLL17, ZYW+16]. oligopeptides [RSL16]. On-the-Fly
[PAK15, MIOM13, PL14, CF18]. On-the-path [CY09, CY13]. One
[MBFP15, CCOH14, GAMAC+14, HRID16, KPL13, LLvG10, LGL11,
LvG13b, LvG13a, PSC11, RPK16, SM16a, SH19, SJC11, SGLH13, WMW+10,
YZZL18, ZZWT12, ZGS+10]. one- [SJC11]. one-bit-per-sample [HRID16].
one-bond [RRK16]. One-electron [MBFP15, PSC11, SGLH13, ZGS+10].
one-parameter [SH19]. one-step [LLvG10, LGL11, LvG13b, LvG13a]. ones
[YZ15b]. ONETEP [LCPS13, WS13]. ONIOM [JAHS+19, AALCM11,
CR19, FBY17, Gil11, GWZX12, Lun12, Mor15, PFAS+19, RJWW12, TS10a].
ONIOM-ccCA [RJWW12]. online [Auo12m, BJP15]. only [LT13]. ONO
[CSKH16]. Open [HLS+13, Aki16, APK14, BG13, FBY+17, HPT17, ISO+13,
KRN+18, KSH+12, NS17, PHT17, RJK14, SRR16, SMRM+17, XTG+11,
Yap11, Yes12, ZCWX18, CZH12, HMO+18]. open-ended [RJK14].
open-shell [BG13, ISO+13]. Open-source [HLS+13, Aki16, APK14,
FBY+17, HPT17, KSH+12, PHT17, Yes12, HMO+18]. opening
[GMBX+16, LGC19, WCL+11, ZQ14]. OpenMM [HLW+17, HLEM18].
OpenMP [JMS14, KS15, KN17]. operation [Bac12]. operational [MA16].
operations [WS13]. operator [LMR14, SH19, SNS13, YLS19]. operators
[Car14, NCT18]. Oppenheimer [BLZ+13, LCH10, RSB+13]. opportunities
Optical [LLX+19, WGL+16, ARLP13, BBL13, BSL10, CJPCT18, GTT10,
HB15, HRJ+14, HRJ+15, JRSHP14, KRTB10, KKPT11, KOP+14, LLB012,
LLD17, MLQ+12, MIS+15, MGS+16, MCK17a, TFQ+10, TFQ+11, TS15b,
YB13, YCGA10]. optically [RJBH18]. optics [Tia12]. Optimal
[DBK17, VSA11, HS12, Kne11b, LTT16, LAT10, LAT11, MLC13, SM17,
Tak11, TBB+10, WGA18, CKH19]. optimally [Ali18, ZZS16].
Optimization [AG11, CB11b, CBI1c, HOK17, LC17b, MY17b, TKN13,
WM12, BW11b, BSD18, BHR15, BW15, BS15, BC13, CY09, CY13, CJI+13,
DS15, DH11, DMAH15, Elk16, GJK+19, HNYH19, HKR12, HJKJ13,
LvDH13, Lch15, LZL+13, LLJ12, Pon10, SA13, SZBM13, SKKS13, SMW09,
SLG15, SR10, SMM17, Tak18, TSQ12, TO10, Vor10, VBV13b, YS15,
optimization-based [YS15].

optimizations [RR12, WX12].

optimized [Boz18, CX10, GA12, HH10, LZZ14, NDW15, NLL19, ŠSB+16, SB14, WO15].

Optimizing [SYDS11].

optimum [KTNN10, SB11, TKNN10, WTD+19].

ORAC [MSC+10].

orange [LWL+11].

orbit [AMQ+14, ATP18, FAA15, FD16, GP11a, JKS+16, KT19, KKA+18, MG11, MCP18, PS17, YB11].

Orbital [SZL19, WM12, ASL+11, Boz18, BVC13, CIKT13, CPN+17, CGPP11, DHF+11, DN19, FE14, GWF11, GLW13a, GLW13b, IIF+10, IKN13, ISM18, KTNN10, LCP13, LFN+10, LTP11, MFR+17, MGS+16, NF18, NPG+18, NF17, OHNK11, OOT15, OOK11, PRY+17, PH15, RKGN10, SGPJS+17, Sch12, SHL+18, SMW09, SB14, SB15, TKNN10, TSH+19, TS14, TSN16, US11, UM13, Wei12a, Wei12b, WCWV15, WM17, ZA15, ZZZ+19, vLBBR12].

orbital-based [CGPP11, MFR+17, Wei12b].

orbital-dependence [SGPJS+17].

orbital-optimized [Boz18, SB14].

orbital-weighted [PRY+17].

orbital/local [SB15].

orbitals [AVHB18, CAF+13, CCM15, Dil15, EP12, Fer13b, Fer13a, GCCM15, HJKJ13, HJJ13, JXSW15, KHLM19, MRB14, MY17a, MBFP15, MCK17a, Sax12, TZ12, VI17, YFI+19, ZR10, ZM11].

ORBKIT [HPT+16b].

ORCA [MG11].

Orchestrated [LL10b].

order [BCCO10, DCHL12, FSSW17, Hil13, KKNN11, KN17, LCL+10, LPS+13, MLQ+12, MCC11, NYH+17, yOTn16, RBOH11, REH13, SK12, ŠSB+16, TAG16, VKAM12, VFRAR16, WLQ19, WHM10, WGA18, ZWF15].

ordered [LPAS11, LC17a, LLB+12, SJZ+15].

ordering [LKZM18, MNNK10a, MNNK10b].

ordering-based [MNNK10b].

Org27569 [ILKR11].

organic [AH10, BBG+18a, Ben17, BE16, BS18, CWHH11, CYG+15, CLK11, DGL+13, ED15, FWS+18, FNSF+11, GLZ17, GAJ+17, KLZ+18, LZ14, LZZ+15a, LWL+10, NPG+18, NDW13, PLZ17, PNW+16, Pog10, PPM15, RSG14, RNS19, SRR16, SH18a, SSNT19, SFDE16, SSAS10, SIG+11, TTR+12, TTB+11, VVV+15b, VVV+18, VVY+11, YJV+11, YNH+17, Zha12a, ZA15, ZCGM11].

organization [AO10, MCC12].

organo [MMS16].

organo-metallic [MMS16].

organocatalytic [ORZ11].

organocuprates [KYCL11].

organometallic [OCLM14, ZYW+16].

organometallics [GMG+10, dCDP15].

organophosphorus [VRKT19].

organoselenium [RK15].

orientation [AST+16, LZ12, LZZG11, RI10, SJZ+15].

orientation-dependent [LZ12, LZZG11].

orientations [WWKS16].

oriented [HPSK12, KG13, RLG14, SCM+15, SK15b].

Origin [FB14a, SB15, CD13, FCOGM12, dLwNC18a].

Origin-independent [ŠB15].

origins [CB11d, NSO+14, WGD+16].

Ornstein [Hei18].

ORP [BLL13].

ortho [LTP11].

ortho-substituted [LTP11].

Orthogonal

[BL15, DC8+15, LAW+16].

orthogonality [GA12].

OsC [ZWW10].

oscillator [LRvdSM15, LM18a, Ric16, SM14b, ZM10].

oscillators [CHC+13].

OsO [ZXS+10].

OSPREY [HMO+18].

other [AFBR17, SK12].
[FBY+17]. PBE [DOM+11, PTK11, LK16a, SGPJS+17, TG12a].
PBE-QIDH [SGPJS+17]. PBE/3z [PTK11]. PBE0
[DOM+11, LK16a, SGPJS+17]. PBE0-DH [SGPJS+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
[HL5+13, Hii13, KD10, Niz13, YDR13, dSdLBNN17, GA19]. PD-PK-T
PDECO [CJL+13]. PDielec [KB16]. PDixCN [ZZL19]. peaks [LZS+17].
PBG [EOO+16]. PEG-PLA [EOO+16]. penalty [GZH10]. penetration
[NLP+16]. penta [LBC+19, Sak18]. penta-coordinated [Sak18].
penta-coordination [LBC+19]. Pentaatomic [XhD15]. pentacene
[CVWH11, ZYG+15, NTN+19]. pentacordinated [TS10b]. pentagon
[FL15, ZYG+15]. pentane [TCGNT18]. pentathienoacene [ZYG+15].
penetration [NLP+16]. penta-coordinated [Sak18]. penta-coordination
[LBC+19]. Pentaatomic [XhD15]. pentacene
[CVWH11, ZYG+15, NTN+19]. pentacordinated [TS10b]. peptide
[FP17a, HPL13, HLH+12, ICS+12, ICS+13, JBAM11, JWST10, LTT16,
LW11, LLvG10, LJJ+11b, LvG13a, LMA15, MDT10, MV17, OZ14, QZM11,
SV15, SEM12, SZB19, TYZ+16, XHLH16, XYZ18, YZ15a, dCLFG13].
peptide-backbone [HLH+12]. peptide-design [XHLH16]. peptides
[BLKP12, BPC13, CR19, COOH14, CZNA11, GFG11, HSB+19, HLH+12,
HHWL17, IO13b, JCR10, KB10, LvG13c, MZZ11, MUGNVJ+18, OLY17,
WNM17, XHLH16, XWSW13, ZKH+10]. peptoid [MMZW14]. perception
[AJR16, HYYZ13]. Performance
[Abr11, BZB+13, CSKH16, CKKK16, DAP+18, DOM+11, GWJR18, HBSB+11,
JCP14, LK16a, RKB+14, SF18, SH18a, SGWA17, ZZMW19, ABM+15,
BLBG+13, CLFR018, CXS10, CSSB11, CJZS10, ESB13, EWK+13, GA14,
GRARO+14, GSS31, HWWL11, KZS+16, KLZ+18, LL10a, LBBD12, LL+10,
MHT+18, MC12, MG11, OPB+12, RRH12, RLS13, SRF+17, SPR+13, SJ16,
TF15, YPC+10, YMY+19, ZHS+18, ZSTRS+18, ZSSL17, ZL13, SBW12].
Pericyclic [HPT16a, KG15, ZZMW19]. period [LOB18]. Periodic
[Sce07, Schul10, AAC+16, BBG+18a, BS18, CMM18, CEBO15, FCD10, Gar12,
HSH15, HBI+17, ITIN15, KB14a, LBGS16, Man13, MG+16, NN18, NO16,
NTN15, RJPB12, RLZ+18, RNS19, SN16a, SP19, Ste15, SPZP18b,
TLdG+12, Tak14, VBB13a, VBB13, VECD12, VI17, YAO18]. Perlin
[HLLBCCG15]. permeation [DMN15]. permutation [IO13b]. pernitrides
[BLKP12, BPC13, CR19, COOH14, CZNA11, GFG11, HSB+19, HLH+12,
HHWL17, IO13b, JCR10, KB10, LvG13c, MZZ11, MUGNVJ+18, OLY17,
WNM17, XHLH16, XWSW13, ZKH+10]. peptoid [MMZW14]. perception
[AJR16, HYYZ13]. Performance
[Abr11, BZB+13, CSKH16, CKKK16, DAP+18, DOM+11, GWJR18, HBSB+11,
JCP14, LK16a, RKB+14, SF18, SH18a, SGWA17, ZZMW19, ABM+15,
BLBG+13, CLFR018, CXS10, CSSB11, CJZS10, ESB13, EWK+13, GA14,
GRARO+14, GSS31, HWWL11, KZS+16, KLZ+18, LL10a, LBBD12, LL+10,
MHT+18, MC12, MG11, OPB+12, RRH12, RLS13, SRF+17, SPR+13, SJ16,
TF15, YPC+10, YMY+19, ZHS+18, ZSTRS+18, ZSSL17, ZL13, SBW12].
Pericyclic [HPT16a, KG15, ZZMW19]. period [LOB18]. Periodic
[Sce07, Schul10, AAC+16, BBG+18a, BS18, CMM18, CEBO15, FCD10, Gar12,
HSH15, HBI+17, ITIN15, KB14a, LBGS16, Man13, MG+16, NN18, NO16,
NTN15, RJPB12, RLZ+18, RNS19, SN16a, SP19, Ste15, SPZP18b,
TLdG+12, Tak14, VBB13a, VBB13, VECD12, VI17, YAO18]. Perlin
[HLLBCCG15]. permeation [DMN15]. permutation [IO13b]. pernitrides
[BLKP12, BPC13, CR19, COOH14, CZNA11, GFG11, HSB+19, HLH+12,
HHWL17, IO13b, JCR10, KB10, LvG13c, MZZ11, MUGNVJ+18, OLY17,
WNM17, XHLH16, XWSW13, ZKH+10]. peptoid [MMZW14]. perception
[AJR16, HYYZ13]. Performance
[Abr11, BZB+13, CSKH16, CKKK16, DAP+18, DOM+11, GWJR18, HBSB+11,
JCP14, LK16a, RKB+14, SF18, SH18a, SGWA17, ZZMW19, ABM+15,
BLBG+13, CLFR018, CXS10, CSSB11, CJZS10, ESB13, EWK+13, GA14,
GRARO+14, GSS31, HWWL11, KZS+16, KLZ+18, LL10a, LBBD12, LL+10,
MHT+18, MC12, MG11, OPB+12, RRH12, RLS13, SRF+17, SPR+13, SJ16,
TF15, YPC+10, YMY+19, ZHS+18, ZSTRS+18, ZSSL17, ZL13, SBW12].
photoionization \[CGP_{12}, MSV_{16}\], photoisomerization \[ZLHH_{14}\], photon \[DPB_{12} + ZTH_{15}\], photooxidation \[LWX_{16}\]. Photophysical \[SCF_{19} + CWT_{12}\], photoreceptor \[XBSS_{19}\]. photoresponsive \[YDGZ_{15}\], photosensitizers \[ZZ_{12}\], photosynthetic \[IIF_{10}\], photosystem \[AKMYB_{18}, KTT_{16}, ZSYH_{12}\], photovoltaic \[NS_{18}\], photovoltaics \[VVMY_{18}\]. phthalocyanine \[SKY_{11}\]. phycocyanin \[RC_{13a}\], phylogenetic \[CCYL_{11}\]. Physical \[CB_{11d}, FCOGM_{12}, JJH_{13} + LHG_{11}, VVP_{12}, YJ_{17}, WCT_{11}\]. physicochemical \[CCYL_{11}, HZY_{10} + LHL_{10}, RI_{10}\]. physiological \[HM_{16}\], phytochrome \[FD_{13}\]. piano \[FPB_{12}, FB_{14b}, ZCK_{16}\], piano-stool \[FPB_{12}, FB_{14b}, ZCK_{16}\]. picture \[ASS_{17}\]. pictures \[MA_{16}\]. PICVib \[dSAdSL_{13}\]. piezoelectric \[ECZWD_{17}\]. pillar \[uLhY_{11}\]. pillars \[NNK_{16}\], pilot \[SSSM_{15}\]. Pimephales \[TTL_{12}\]. pinane \[BLS_{10}\]. pincer \[ED_{15}, JJA_{16}\]. pincers \[KJDB_{12}\], pincer \[HJJ_{13}\]. pivoting \[PS_{17}\]. PK \[HLS_{13}, GKI_{15a}, SKI_{15a}, SKI_{12}, SKI_{17}, YDX_{16}, Zha_{12b}, Zha_{12a}\]. PKA \[MUGN_{18}, EOO_{16}\], Placevent \[SYH_{12}\], planar \[BSP_{13}, LVI_{14}, KSO_{19}, XD_{15}, YS_{18}, YLZ_{16}, YZW_{17}\]. planar-chiral \[KSO_{19}\]. planarity \[NK_{19}\], planarization \[NK_{19}\]. Plane \[SH_{14}, BTB_{11}, EHI_{13}, Gav_{12}, LL_{13b}, MDT_{13}, MDT_{16}, TCP_{16}\]. Plane-wave \[SH_{14}, BTB_{11}, MDT_{13}, MDT_{16}\], planewave \[SM_{18}\]. planning \[FBvdB_{18}\], plasmepsin \[SOD_{11}\], plasminogen \[BM_{12}\]. plasmogen \[Ano_{15-58}, BH_{14}\], plastocyanin \[HBI_{17}\], PLATform \[TN_{16}, BTM_{12}, HPT_{16b}, PSG_{17}, PZC_{16}, VM_{17}\]. platforms \[KJ_{17}, SC{OJ}_{13}\], platinum \[ITY_{19}\], platonic \[KSM_{16}\]. PLATYpus \[TN_{16}\], plausible \[KV_{14}\]. Plested \[FSSW_{17}, HII_{13}, KKN_{11}, KNI_{17}, MCC_{11}, YKH_{15}\]. PlmII \[VLB_{10}\]. PlmII-inhibitors \[VLB_{10}\], plot \[MP_{17a}\], plug \[BTA_{13}, KLS_{10}\]. plug-in \[BTA_{13}, KLS_{10}\], plugin \[FRC_{18}, RD_{18}, BHB_{12}\]. plumbacyclopentadienylidenes \[KASH_{14}\], PM3 \[SA_{10}\], PM3-CARB1 \[SA_{10}\]. PM3-CARB1/Tip3P \[SA_{10}\], PM6 \[SBW_{12}\], PM6-DH2 \[SBW_{12}\], PMF \[ZLX_{13}\], PMI-MDM2 \[HQSZ_{19}\]. PMMA \[NSS_{15}\], pnum \[GMS{Gd}_{15}\]. nicipogen \[L{DG}_{15}\]. Pocket \[AIM_{18}\], pockets \[MK_{11}, TN_{17}\]. Point \[Lar_{11}, AS_{15b}, AGM_{13}, BHR_{15}, BTL_{11}, BTB_{11}, EPD_{10}, LPS_{12}, LLWS_{14}, OHPR_{17}, SN_{15}, Tc_{17}, TBSM_{12}, We_{12b}, YHW_{17}, dLvN_{18}, NQB_{19}\]. points \[HD_{17}, HEMC_{14}, OHPR_{18}\]. Poisson \[ALRM_{18}, BCCO_{10}, BD_{12}, CLA_{16}, FBY_{17}, FHMB_{15}, FCE_{15}, FBvdB_{18}, Fra_{15}, Fra_{16}, GRARO_{14}, NW_{17}, SK_{15a}, WL_{10}, WLQ_{19}, XXY_{17}, YOMT_{14}, HWL_{11}\]. polar \[BK_{17a}, CVG_{14}, GMG_{10}, L{V}_{13b}, PAT_{10}, WWW_{18}\]. polar-nonpolar \[WWW_{18}\]. polarizabilities \[BLBG_{13}, BZB_{13}, KR_{12}, KNP_{12}, LIRL_{16}, ML{C}_{13}, PL{F}_{18}, RLA_{11}, SS_{16b}, XKW_{18}\]. polarizability \[CPK_{12}, EPD_{11}, H{BKL}_{10}, KS_{11}, N{YN}_{17}, OVP_{15}, PC_{14}, YB_{13}\]. polarizability/reaction \[K{S}_{11}\]. Polarizable
[CCR18, GEP +14, LM18a, LPS +13, LCL +18, NS11, SAvG15, ZM10, ALRM18, BSL +16, Cam15, CCB15, CGPP11, DGM14, DGB +13, DDM +15, ENKK +17, ESM +12, FP17a, GRS15, GpdC +16, HOK17, HZSS17, HLEM18, HCP15, ISO +13, KFY +13, KR12, KW1 +16, LRvdSM15, LFN +10, LHHW14, LDG +15, MBC11, MBC13, MBE16, NLP +16, ODB18, PMC17, PZCL16, Ric16, SM14b, SK17, SBvG14, VVLG17, WRHF10, WLO +17, XZ11, XP13, ZRL +15, ZP13].

Polarization [Mit13, CD11, JZ12, LOB18, LCW12, MLZZ14, POB13, RF15, TNG +10, WWD14, YD17, ZJZM13, ZBG11, ZBP11].

polarizeable [SS16b].

Polarized [BS10a, B LG +13, DLZ15, JZZM14, NHF +10, SFM14, SEJ +18, VHS +19, YJXZ13].

pole [NYN17].

polarization [GCC14, SIG +11, TTR +12].

pollution [LZ14].

poly [CH10, PRRT +10].

polyacenes [KAR12, RS17a].

polyacetylenic [ZZZ +19].

polyamidoamine [CAD16].

polyatomic [OT12].

polybrominated [GKR13, Ray13, RKG11].

polycyclic [CB11d, FVB10, Kar17, PL18, ZWX19].

polyelectrolytes [NSP15].

polyethyleneimine [BAF18].

polyethylenimine [BF17, MT19a].

polyglutamine [CCOH14].

Polygonal [PL18].

polyguluronate [Pla11].

polyhedra [CD16].

polyhedral [CL16].

Polymer [HP10b, PH10a, AHK +19, KZP +18b, MZZ11, SCMA +17, YCGA10, YFH +19].

polymer-growth [MZZ11].

polymer-stabilized [AIK +19].

polymerase [SBT17].

polymerization [KZP +18a, MTS +19, SCK18, YMY +19].

polymers [CRC13, GRE11, KLZ +18, SA11].

polymorph [SPZP18b].

polymorphic [SLY +10, XWSW13].

polymorphisms [LXZ +11].

polymorphs [RRC +15, WRM +12].

polynomial [SY11].

Polynuclear [SVLK18, CAT +13].

polyoxometalate [JAHS +19].

polyoxometalates [CB11a, CB11b, CB11c, GLZ17, RDF +11].

polyoxy [SC18a].

polyoxy-anion [SC18a].

Polypeptide [AD10, IUK +11].

polyphenacenes [QZ10a].

Polyphlic [vRWGS17].

polyaccharide [KSW16].

polyspherical [PH10a].

polyuronate [PD12].

poor [HDH12].

popular [CXD +19].

populated [CBP +15].

population [LTA +11].

population-based [LTA +11].

Populational [DK11].

populations [BVC13, KV13, OGL10, VZ14, WES13].

pore [KJ10, SBFT17, WNM17].

pores [DMN15, Fom13, HPL13, LJR +12].

porous [LZ14, PLZ17, SYZ +17].

porphin [SMDP18].

porphyrin [BEL +11, EH13, INT18, KCK +15, PLZ17, VBA13, FAS +18].

porphyrins [MLQ +12, TSNC +17].

portable [KS13a].

Porting [WS13].

pose [Vor10].

poses [HWWL11].

position [LHO17, VDVR14, BEEL14].

positions [AVHB18].

positive [SRA17, VVY18].

positron [SS +18].

positronation [BL12].

Possible [Oht16, FHK +12, GNI18, RB12, Tsi17, NJR18].

POSSIM [LPS +13, SK17].

post [BY11, CGR16, CB11d, MRO17, RRH12, SJL18].

post-Hartree [CB11d, RRH12].

post-MP2 [CGR16].

post-self-consistent [BY11].

post-translationally [MRO17].

Post-treatment [SJL18].

postprocessing [HPT +10].

potential [NS10, XDL +10].

Potential [KIOY19, OSI +19, SC17, Vor12, AMGB10, AS18, BTA +13, BLF14, BT18]
primary [ALK+15, GA13, VVLG17, KTNN10]. prime [DSX+11].

prime/MM [DSX+11]. primitive [HAL14]. principal [PSP15]. principle [CCJC10, DBM+15, LLB+12, MCF10, SBGP18, Tak11, YPyD13]. Principles [HFSO12, BE12, BE14, BPE16, EMD17, EB12, EBK13, EBPK17a, EB18, GD10, HYL+11, Ib17, JCG+11, KLZ+18, LLLM11, LCWW10, NNS15, PLZ17, RGZ+13, SFA17, SPZP18a, TZ11, UGK18, WYL+15, WD10, YR13, wZbZ11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC+14, THI+19].


PROCOS [FHW+11]. produced [LS11a, SIG+15]. Producing [RN17].

product [CC12b, ZQ14]. production [GYX+10, SSNT19]. products [KIOY19, TR12]. profile [AK10, BS16a, GTZ+18, KTT16, XML+15]. profiles [MIOM13, RB0H11, SISK10, Yl12b]. profiling [VMRSH+17].

profit [KB11c]. Program [FPV13, GH16b, SWA13, BBG+11, BBG+18b, CBH14, CZZL19, CAT+13, FM10, GLW13a, GLW13b, GBW+14, HS16a, HSN+18, HL14, JS17b, KWL+16, KK17b, LHS12, MHT+18, MSC+10, MSvG12, Mez10, MSP17, MAP18, MB14, NMMH19, SMPD18, SFG+17, SFR+11, SYN+12, TNT16, TSC+13, UDK+18, VV15+15, WDCM11, WHK+12, ZL11].


proline [AS11, HJLV16, OOK11]. proline-catalyzed [HLV16].

proline-recognition [OOK11]. promelas] [TTL+12]. promising [KSSH13, RNS19, ZSSL17]. promolecular [REV+17]. promoted [LPLB16, QXY+18].

Proof [FVB10]. propagator [WWD14, YLS19, YD17].


propene [HSL+11, QSW+10, dSddAR10].

Properties [LLX+19, MP19a, SFCCK+14, TY10, AWF+18, ARAG17, ASS10, Avd18, ARLP13, ALH+10, BCSCJ+13, BE12, BPE16, BLFZ13, BS10a, BAD+19,
BP18, BACSCJ+10, BC13, CPRS18, CBH14, CWT+12, CWHH11, CBTZ16, CH10, CCY11, CCS10, CLC11, CJPTC18, DDP16, DOM+11, DMD+18, DBM+15, DPNM11, DJX+11b, DJX+11a, DP15, DLW12, DQ16, EPH+15, EBPK17b, FB10, GBL+11, GTT10, GK10, GNI18, GWWJ12, GBGR16, GBG+19, HZY+10, HR3+17, HLH+12, HZSS17, HLWD15, Ibr17, JBSQC11, JH+13, KKT11, KDB13, KZK+12, KPG18, uLhY11, LHL+10, LSHH12, LLM11, LZJ+11, LLD17, LBTV12, LZX+10, LWG12, MC10, MCF10, MJLV14b, Mat10, Mat14, MIS+15, MGS+16, MCK17a, NC14, NS18, PGC13, PGY15, Pog10, PH10b, Pop18, PBE16, PS10, RR14, RRF11, RI10, SDF+17, SCF+19. properties [SB11, SIT18, SLIB12, SWMW10, SZB19, SIG15, SGH+16, TN12, TFQ+10, TFQ+11, TS11, TS15b, VVW+18, VPR10, VECT12, WLC12, YW12, YCGA10, ZYG+15, ZWMW10, ZB18, ZLX+13, ZBP11, ZYL+12, FDCJG18, SFCCK+15]. property [CD13, GPS10, GBS+17, GWX+12, PH15, V˚AA14, WH11].

propionate [TN10].

propanoate [NC14, NS18, PH10b, Pop18, PBE16, PS10, RR14, RRF11, RI10, SDF+17, SCF+19]. properties [SB11, SIT18, SLIB12, SWMW10, SZB19, SIG15, SGH+16, TN12, TFQ+10, TFQ+11, TS11, TS15b, VVW+18, VPR10, VECT12, WLC12, YW12, YCGA10, ZYG+15, ZWMW10, ZB18, ZLX+13, ZBP11, ZYL+12, FDCJG18, SFCCK+15]. property [CD13, GPS10, GBS+17, GWX+12, PH15, V˚AA14, WH11].

protease [DLZ15, NHN16, OBW12, SYH12]. protection [SBW12].

protective [JAH+17]. Protegrin [RI10]. Protegrin-1 [RI10]. Protein [CIKT13, CDS16, DPOS16, GPS10, HTS15, HS16b, LZGS11, MEFM16, MFR10, PGL+15, Ran12, RP15, Rao11, SHMO11, SKKS13, AIGP15, AKK+16, AM10, AG12, BZS+12, BFH+13, BB11, BCP13, BCG10, Bow16, BDD13, BA11, CFA+18, ZAF17, CFC15, CHR+12b, CHR+12a, CM13b, CCYL11, CKP10, CH14, CC12b, CBG16, CHP11, DL11, DJ13, DRV14, DLMH12, ESD18, FZY+12, FHW+11, FCE15, FLM11, FSC+14, GS14, GGD17, GMSdG15, GRP+12, GZ14, GRL+11, GRL+12, HAGK10, HNNR13, HMO+18, HTS15, HTS17, Has14, HZY+10, HPL+18, HKR12, HYMZ16, HJ10, HHHY10, HM13, HZ13, HQS19, ILKR11, IHY15, JZ12, JZM14, JZL+17, KTE+17, Kan15, KNE11a, KNY+12, KL14, KERY+16, KJ10, KTO11, KTO13, KDT+12, KLS10, KMLS10, LS11a, LFB14, LHL+10, LH11, LCP13, LC16, LC17b, LZ11, LLC+10, LI10b, LFM12, LPS+13, LZU14, LLLC11, LH11, LBS10].

protein [LM18b, LDH+14, MS17, MMM+16, MJC14, Mau14, MUGNVJ+18, MA17, MEFM15, MS16, MP11, MKB+13, MOS12, MNNK10a, NSK18, NS14, NS11, NFG+13, NG10, OHNK11, OCL11, OL13, OBW16, OCLM14, OK16, OME16, OOT15, PGCT+12, PGW+17, PLV+11, RZZ+13, RCR+16, RMRBH+19, SPP+18, SBB10, SYDS11, SK17, SGG+18, SM13+13, SY16a, Sti15, TYZ+16, TNY16, TCC+18, TNSS17, TRA+16, TJB12, UNT16, UC1F16, VMPS17, WDVN12, WNP+16, WZ17, WLLH18, WES13, WHAS+10, WHAS+16, XML+15, YXZ18, YZ15a, YZ16, YDL+10, You16, YS10, YL13, ZC14, ZYvZ14, ZLW10, ZLX+13, ZDT18, ZSB+16, dRBO13, AIM+18, DKV18, LGL11, SL10, SHL+11]. protein-bound [FLM11]. protein-coding [YS10]. protein-coupled [ILKR11]. protein-jaundice [AG12, CH+12b, CH+12a, LLC+10, OOT15, SPL+18, WDVN12, dRBO13, AIM+18]. protein-like [KOY+12]. protein-lipid [PGCT+12]. protein-peptide [XYZ18]. Protein-protein

retinal [CG12, GA18, SGWA17, WGA18, ZLHH14]. retinoic [LFM12].
Self-guided [WBVE16, OCL11]. self-guiding [HS17a].
self-interaction [SHL18, TSH19, vS18]. self-metathesis [MJL14a].
semi [DAG19, FSSW17, SC15]. semi-direct [FSSW17]. semi-empirical
[DAG19]. semi-global [SC15]. semiclassical [YLS19]. semiconducting
[VS14, ZSLL17]. semiconductor [LCH15, SFDE16, VVMY18].
semiconductors [BE16, NDLW13]. Semiempirical
[FA18, SRL15, BP18, GKL19, GP11a, HG15, KTNN10, KB14b, LSD10,
MGWR12, SPH11, SDL14, TKNN10, TG12a, UCFR16, WCWW15].
semielementary [VDVR14]. Seminumerical [PW12]. sense
[DR14, ICS12, ICS13, NH19]. sensing [LZL10, LCC18, RRK14].
Sensitivity [Han11, LL11, LWWG12, PDG16, Sea10]. sensitized
[ACS12, JYS12, LZL15a, YJN11]. sensitizers [YJN11].
sensitized [ACS12, JYS12, LZL15a, YJN11]. sensitizer [YJN11].
sensitizers [SLC17]. sensors [DHE12]. separable [WWU12]. separated
[Ali18, BK17b, HZSS17, RSG18, SH18a, SZZS16, WYT17]. separation
[CSKH15, DS12a, NMH19, VCL18, VL17b, YSG12]. Sequence
[TYZ16, DLI10, DNL11, HPL18, LXL11, MP17b, RMRBH19, Sti15,
TYX18, WXL12, YZWC11, YS10, ZWP11, HYMZ16]. Sequence-based
[TYZ16, RMRBH19, WXL12]. sequence-reactivity [Sti15].
Sequence-specific [HYMZ16]. sequences [Ano12u, CCYL11, Fel10,
HZY10, LML11b, LLVM11, LDH14, OLA15, QLQ11, YDL10].
Sequential [CBP14]. sequestration [CC18c]. Ser [LY10]. Serenity
[UDK18]. serial [BB11a]. series [AWF18, AC11b, DDM15, FWS18,
LZGS11, MCK17b, SB10, TD10, AM19]. server
[CPA11a, XML15, XYX18, dVAG16]. servers [UHH11]. services
[LP11a, UHH11]. Set
[SN16b, BLL13, BGL10, BLRS08, BRLS12, CC11, HS16b, KNP12,
LS11a, LLC10, LVC13, LZ18, LW110, Mat10, OAN15a, PML12,
PG10, PHK14, PD11, Pog10, PFVL14, RLD12, SPS12, Sch13, SWM10,
SG10a, SG13, VLGK17, VVLG17, WX12, YOMT14, ZPP16, FL15].
Sets
[TKN13, BLFZ13, BLBG13, BLF14, BS10a, DBM15, HSN14, H113,
LOB18, LBH11, LCW12, Leh15, Mit13, PO13, Sea10, SNKS10, ST15,
TH13, UCFR16, ZLT13]. Setschenow [XWW11]. setting
SG-3 [DH17]. SH [XCLZ19]. SH2 [AC11a]. Sham [BWMS10, SS16,
VV14]. Shao [Ano12u]. Shape [KC14, Zha11, GPS10, HCB11, Hsu14,
MNNK10a, OAN15b, XTY14, YLGCX14]. Shape-based [KC14]. shape-complementarity
[GPS10]. shaped [LWZ13]. shapes [KC14, PL18]. Shared
[vW11, UWI10]. Shared-memory [vW11]. sharing [JSF19]. shed
[GN18]. sheet [CCOH14, Hug12, WS10]. sheets [PL18, WCAH10, YZZ17].
shell [BH14, BG13, GKSS14, ISO13, JCG11, KSR17, MBA11, MA16,
MS12, SRR16, TBSM12, TEDT18, WWD14, Ano15-58]. shell-wise [KSR17].
shells [GPK12, JXS15, SC18a]. Sheppard [QB11]. shielding
[GMSV14, HAI16, FC14, VAMS14, YS13]. shellings [JKS16]. Shift
LWZ$^{\pm}19$, LBDP$^{12}$, MCvdV$^{13}$, MSC$^{\pm}10$, MBR$^{\pm}$15, MTS$^{\pm}19$, MSvG$^{12}$, Mez$^{10}$, MMZW$^{14}$, MLCD$^{11}$, MCC$^{12}$, NPG$^{17}$, NFG$^{+13}$, NDD$^{+10}$, OYK$^{+11}$, ON$^{14}$, PLZ$^{17}$, QLKI$^{19}$, RHNN$^{10}$, RAR$^{+11}$, RO$^{14a}$, RO$^{14b}$, RSR$^{+12}$, RSLS$^{13}$, SWM$^{10}$, SK$^{15b}$, SMRM$^{+17}$, SSP$^{19}$, SHL$^{19}$, SS$^{19}$, SJZ$^{+15}$, SBvG$^{14}$, SAvG$^{15}$, TNYN$^{16}$, UTM$^{11}$, UU$^{12}$, VMRS$^{+17}$, Vor$^{12}$, WC$^{11}$, WLF$^{19}$, YAS$^{13}$, ZX$^{11}$, ZSS$^{+13}$, ZKH$^{+10}$, ZLL$^{+13}$, dCLFLGL$^{13}$, SG$^{18}$. **Simulations**

[BRE$^{16}$, MFEM$^{16}$, PK$^{19}$, RJH$^{18}$, RKDM$^{14}$, XFG$^{+16}$, Aki$^{16}$, BTA$^{+13}$, BM$^{12}$, BDTP$^{11}$, BW$^{15}$, BF$^{17}$, BJP$^{15}$, MBMJ$^{11}$, BB$^{11b}$, BB$^{11c}$, BBI$^{+11}$, CTR$^{13}$, CCOH$^{14}$, CVG$^{14}$, CLK$^{11}$, DGH$^{+11}$, DMN$^{14}$, DSD$^{+11}$, DHF$^{+11}$, DZT$^{11}$, DLZ$^{15}$, DDM$^{+}$, ER$^{18}$, EK$^{15}$, FTW$^{12}$, GBL$^{+11}$, GR$^{11}$, GPM$^{17}$, GCW$^{14}$, GP$^{11b}$, Has$^{14}$, HCD$^{10}$, HFSO$^{12}$, HPSK$^{12}$, HDPM$^{14}$, HMM$^{10}$, HYUS$^{11}$, HJ$^{10}$, HHWL$^{17}$, HLEM$^{18}$, HI$^{18}$, IPAA$^{11}$, JIS$^{13}$, JWO$^{15}$, JMS$^{14}$, KV$^{13}$, KCK$^{+17}$, KCK$^{+15}$, KvdV$^{14}$, KGK$^{12}$, KGC$^{15}$, KLOS$^{10}$, KBI$^{11a}$, KTO$^{11}$, KSR$^{+16}$, KLS$^{10}$, KMLS$^{10}$, KZP$^{+18a}$, KW$^{+16}$, KV$^{15a}$, KPF$^{+15}$, LH$^{11}$, LC$^{17a}$, LRvdSM$^{15}$, LZ$^{12}$, LPS$^{+13}$, LMI$^{+14}$, LZLMP$^{16}$, LCL$^{+18}$, LM$^{18b}$, LAS$^{+14}$, MMH$^{19}$, MN$^{15}$, MCR$^{17}$, MTvG$^{12}$, MFEM$^{15}$, MADWB$^{11}$, MAP$^{18}$, MKM$^{+17}$, MB$^{14}$, NST$^{14}$, NFPD$^{13}$, NNK$^{+16}$, NTNY$^{15}$, Oht$^{16}$, OCL$^{11}$, OLY$^{17}$, OZ$^{14}$, OCW$^{+15}$, PGY$^{15}$, PH$^{17}$, PZCL$^{16}$].

**Simulations** [PL$^{14}$, PM$^{13}$, PS$^{13}$, PS$^{10}$, PNG$^{10}$, RD$^{18}$, RdA$^{12}$, RLG$^{14}$, RSR$^{15}$, SSO$^{19}$, SBV$^{10}$, SS$^{13b}$, SHFJ$^{18}$, SB$^{T}^{17}$, SISK$^{10}$, SCK$^{18}$, SJ$^{17}$, SMP$^{17a}$, SYN$^{+12}$, SK$^{13}$, SFLG$^{+17}$, SB$^{15}$, SWB$^{+12}$, SDMS$^{13}$, SV$^{11}$, VSA$^{11}$, VKT$^{15}$, VM$^{11}$, WKL$^{12}$, WAM$^{17}$, WH$^{11}$, WWA$^{11}$, WLC$^{12}$, WBF$^{17}$, WG$^{14}$, WO$^{n18}$, WC$^{J}^{+14}$, XFG$^{+15}$, XWS$^{13}$, YKO$^{+11}$, YSG$^{12}$, Yon$^{16}$, YHV$^{12}$, YFH$^{+19}$, ZZY$^{+16}$, ZDKM$^{12}$]. **Simulator**

[BSL$^{11}$, KJM$^{+17}$, RLLHL$^{12}$, TCX$^{+13}$]. **Simultaneous** [LL$^{10b}$, WZZW$^{18}$].

**Single** [HPL$^{+18}$, LP$^{11c}$, PM$^{18b}$, SR$^{18}$, Zim$^{15}$, AS$^{15a}$, BE$^{14}$, BP$^{18}$, BK$^{17b}$, Den$^{12}$, FTR$^{15}$, GCCM$^{15}$, K$^{K}$, KJ$^{G}$, LXL$^{+11}$, MS$^{Y}$, MT$^{19b}$, MCLD$^{10}$, MEH$^{18}$, PBE$^{16}$, RHNN$^{10}$, RLD$^{17}$, SY$^{16b}$, TSR$^{+16}$, VS$^{14}$, WL$^{+10}$, WYL$^{+15}$, YZN$^{13}$]. **Single-** [BE$^{14}$]. **Single-bond** [GCCM$^{15}$].

**Single-configuration** [MT$^{19b}$]. **Single-ended** [Zim$^{15}$]. **Single-excitation** [ME$^{18}$]. **Single-file** [SY$^{16b}$]. **Single-ion** [BP$^{18}$]. **Single-pass** [SR$^{18}$].

**Single-sequence-based** [HPL$^{+18}$]. **Single-step** [RLD$^{17}$].

**Single-vibronic-level** [MCLD$^{10}$]. **Single-wall** [KG$^{19}$, TSR$^{+16}$].

**Single-wall** [AS$^{15a}$, PBE$^{16}$, VS$^{14}$, WYL$^{+15}$, YZN$^{13}$]. **Singles** [EK$^{17}$].

**Singlet** [BSDP$^{16}$, HWB$^{19}$, ISO$^{+13}$, RS$^{17a}$, SSC$^{+19}$, THP$^{+15}$, TCPPC$^{14}$, NNT$^{+19}$, ZSL$^{19}$, ZZL$^{19}$]. **Singlet-triplet** [RS$^{17a}$]. **Singlet** / [ZZL$^{19}$].

**Singular** [Les$^{19}$, SG$^{10a}$]. **Singular-value** [Les$^{19}$]. **SiO** [DOM$^{+11}$, HEM$^{+17}$].

**SiOH** [LvDH$^{13}$]. **SIPs** [KCC$^{+18}$]. **Site**

[CH$^{14}$, LJW$^{+11b}$, CVG$^{14}$, DAP$^{+18}$, GEP$^{+14}$, GPdC$^{+16}$, HL$^{14}$, ISP$^{+10}$, LB$^{+12}$, LKZ$^{18}$, LL$^{+12}$, MP$^{13}$, MNNK$^{10a}$, OHP$^{17}$, OHP$^{18}$, RLD$^{17}$, SHF$^{11}$, SB$^{11}$, SC$^{18b}$, TYN$^{15}$, ZLX$^{+13}$]. **Sitedirected** [CH$^{14}$].

**site-identification** [RLD$^{17}$]. **sites** [AIGP$^{15}$, An$^{12u}$, DVVP$^{14}$, DBK$^{17}$, JAH$^{+19}$, KDT$^{+12}$, LZTV$^{10}$, LHL$^{+10}$, LL$^{10b}$, LZX$^{16}$, LG$^{14}$, MA$^{16}$, PHC$^{13}$, PGB$^{17}$, TYZ$^{+16}$, TYX$^{+18}$, Vor$^{10}$, YZ$^{15a}$, YHH$^{+13}$, ZZL$^{+12}$]
[ZJL+17, LZY12b], six [DOM+11, XhD15]. Size
[Tak18, AS15a, BLBG+13, BD12, CC12a, CF14, DJX+11b, FE14, GZZ12, Hsu14, MTVg12, SL17, SB11, XYX17, Zha11, NNT+19]. Size-guided
[Dil15, LRER13, MY17b, SFG+17]. Slater-function-based [SFG+17]. Slater-type [Dil15, MY17b]. slices [AKN16]. slicing [KCC+18]. SLIM
Smoluchowski [KS18, SG10a]. smooth [AG11, EFS16, JLCA17, ZSB+16]. smoothed [LZ12]. SMPBS [XYX17]. Sn
[MCK17b, PMG+16, RDT14, YW12, AS10, PKK17]. SnCl3 [dSDdAR10]. SnO [DHE+12]. Sodium [KL16]. Soft [SJC11, Ben17, BG12]. Soft-core
[SJC11, BG12]. Software
[AIGP15, Aki16, APK14, AAC+16, BTA+13, BHB12, BCSCJ+13, BSZ+12, Ber17, BJP15, BFI+13, BBG+18b, CBH14, CSEMB+16, CZAF17, CAT+13, DM15, DJD12, DVVP14, DBDP16, DDK14, DWC17, DSK17, ESB13, EWK+13, FN12, FSC+14, GMSdG15, Gar12, GJMPAM+14, GLW13b, GS12, GCP+13, GCC14, GBW+14, GH16b, HLS+13, HRB+17, HD12, HPT+16b, HPSK12, HHT+13b, HH16b, HG13, HYMZ16, HKR+14, HBJ+17, HL14, HC14, IGK16, JHH+13, JJW+14, JLCA17, JP15, JCGM18, KS13a, KS15, KK17a, Kan15, KR14, KB16, KKR+13, KDR+18, KLJ+17, KMM+17, KDT+12, Kos16, KG13, KWL+16, KK17b, KWG15, KSD+12, KYG+15, KAG+12, KSW16, KPF+15, LPS12, LJR+12, LHS12, Leh15, LRvdSM15, LRvE17, LDB+17, LLZA12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MTD16, MBR+15, MTK18, MSSP17, MB14, MB16, NKK16, OV14, OPB+12].
Software [OZS+13, OC14, PSS14, PGL+15, PSG+17, PW12, PPM15, PHH+12, PVZ13, PG14, RLLHL12, RNSF+16, Ras17, Rez16, RR14, RdA12, RSR+12, RCN+13b, SM14a, SFG+17, SK15b, SWA13, SRM+17, She12, SCI, SIE15, SJ17, SVLK18, SWB+12, SDMS13, TNYN16, TSC+13, TTL+12, UU12, VMRSH+17, VVV+15b, VAR12, VBV13b, WDVN12, WDI13, WPM+15, WF16, Wei12b, WHK+12, WJJH13, WG14, WCJ+14, XML+15, XYX17, YWJ+16, YZ16, Yes12, Yes15, YHH+13, ZDKM12, ZLL+13, dVAG16, CCC+11, DBF14, EdOdS18, FRC18, HSW+19, MSvG12, MJG+15, SF18, SBV10, SGM+13, Yap11, ZCS+15, She12, SJL18]. softwares
[All11]. solar
[ACS12, DGL+13, JYS+12, LZZ+15a, SL+17, TZ12, VAA14, YJN+11].
Solid [MP19a, RSK+15, ASS10, ASK18, CL16, HLS12, HBI+17, KLN12,
KKH18, LOB18, POB13]. **Solid-state**

[RSK15, HBI17, KLN12, KKH18, LOB18, POB13]. **solids**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BRLS08, BRLS12, EOA11, RVM19, TKT11, YKO11, Yan11]. **solute/solvent**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**

[BK11, HAI16, MDTD13, MS15, dlRL11, Pon11, SN16a]. **Solubility**

[MSY19, KKO16, WZW18]. **solute**
Specific

[CBP+15]. **Sparsity** [HNS16, BYE+16, RR11]. sparsity-exploiting

[BYE+16]. **Sparsity-weighted** [HNS16]. **Spatial**

[PTB+15, HAL+14, MVG12]. **SPC** [GM17]. **SPC/E** [GM17]. **SPC/E-I** [GM17]. **special** [Alg+14, MG11, OSS10, RH+15, SSA+17, TCPCC14, Ts14, VRK+19, WvR+14, ZZ10, ZLY+16].

**Specific**

[DHF+11, OHNK+11, CIKT13, CCM+15, GCCM+15, HN+19, HY+16, JJZ+14, KR+12, LHO+17, LGL+11, LF+17, MCC+11, MC+12, SSS+15].

**spectrality** [LJW+11b, LBS+10, ZK+11]. **Spectra**

[PAK+15, TT+18, AMQ+14, BG+17, DCOD+13, EBPK+17b, FD+13, FF+11, GWF+11, GGM+12, GZ+17, HRH+17, KASH+14, Kow+11, LC+12, LX+11, MAK+14, ML+10, MKK+19, NHF+10, PMR+17, PDMT+10, PDR+16, RS17a, RI+17, SGT+10, SB+15, SR+11, TYN+15, TZC+18, TG+12b, Ts14, WGL+12, WW+14].

**spectral**

[Ano+58, BH+14, HRM+13, KZZ+16, NSO+14, QZM+11, RLG+11, SF+16].

**spectrometer** [LBB+15]. **Spectroscopic**

[SS+13b, GKh+10, KDB+13, KOp+15b, NC+13, NC+14, TZC+18, Ts14, ZL+10].

**spectroscopy** [DM+18, HPSK+12, IY+18, KN+18, LLB+12, Lin+18, NC+12, WH+12, FAS+18]. **spectroscopy-oriented** [HPSK+12]. **spectrum**

[BLF+14, KCC+18, MN+19, ML+11, RDF+11, SLL+13, TSC+13, ZD+11].

**spectrum-slicing** [KCC+18]. **speed** [MSR+18]. **speed** [TO+10, VM+11, YD+17].

**speed-up** [YD+17]. **speeding** [AO+10]. **spalerite** [SBC+11]. **sphere**

[KT+12, MH+10, Pop+18, TH+13]. **spheres** [HS+16b]. **spherical**

[Ano+58, BH+14, YOB+16]. **spherically** [YOB+15, Yvb+16]. **spheroidal**

[ZWY+10b]. **spider** [Che+17]. **SPILLO** [DVVP+14]. **Spin**

[AT+18, DSM+11, JKS+16, KM+13, MLG+18, TT+18, AB+10, AMQ+14, CSE+16, CSS+17, CSK+16, CAP+17, FAA+15, FD+16, GP+11a, KT+19, KIO+19, KSK+11, KKA+18, LFX+17, MG+11, MCP+18, PLF+18, PS+17, RRK+16, SF+14, SPH+18, SB+16, SH+18b, TN+18, TN+19, VFR+16, VHS+19, YB+11, ZL+14, ZZZ+19, S+19]. **Spin-component-scaled** [KM+13].

**spin-coupled** [SH+18b]. **Spin-driven** [DSM+11]. **spin-flip** [ZL+14].

**spin-forbidden** [TN+18]. **Spin-orbit** [AT+18, JKS+16, AMQ+14, FAA+15, FD+16, GP+11a, KT+19, KKA+18, MG+11, MCP+18, PS+17]. **spin-orbital** [ZZZ+19]. **spin-polarized** [SF+14, VHS+19]. **spin-rotation** [KIO+19].

**spin-spin** [PLF+18, SPH+18]. **spin-symmetry** [TT+19]. **SPINE**

[FZ+12]. **Sinor** [CC+12b, BA+14]. **spins** [ZR+10]. **Spiral** [SK+8]. **Splitting** [Rob+13, EHS+16, FL+19, LL+19, OT+12]. **SPME** [NL+16]. **SPOT**

[YZZ+16]. **SPOT-Ligand** [YZZ+16]. **spots** [HSQ+19]. **Spread** [BE+14].

**squaraines** [AMQ+14]. **square** [HDL+14, HGW+18, ISK+14]. **squared**

[JMS+13]. **squares** [BCC+10]. **SR** [AR+17, WM+11]. **SR-ZORA**

[AR+17]. **SrO** [BL+12]. **SSC** [LG+11]. **SSThread** [Mau+14]. **ST** [JJW+14].

**ST-analyzer** [JJW+14]. **STAAR** [JHH+13]. **stabilities**

[BL+13, SIT+18, TFQ+11]. **Stability**

[CS+16, EK+17, GWT+17, Ld+16, Lin+18, OME+16, PP+10, BPP+17, CSS+17,
CFC15, CM16, CB11d, DLT17, DLW12, GPK+16, GC18, Ham11, HLB15, LTR18, LHK512, MC10, MS15, PMG+16, PAT+10, Rab12, SBGP18, SY16a, SPZP18a, TN12, TKCN19, XFTW15, ZRCC11, ZWMW10, ZWW10.  
Stabilization [KSR17, BSDP16, DBK17].  
Stabilize [KG11].  
Stabilized [AHK+19, KASH14].  
Stabilizing [MvBD18].  
Stable [NPTS16, PBDW11, ZDZM13].  
Stacked [ANH+11, HvM12, LDH+14].  
Stacking [HvM12, YZZ+17].  
Stages [CBP+15].  
Standard [DH17, BCJC+14, MKO+13, PNI13, RD18, REL+14, SRR16, VVG13, WHK+12, WGA18].  
Standing [TS11].  
Staple [SV15].  
Star [MA17].  
State [CCM15, FHG+19, GS16, MP19a, TT18, Alg17, AR10, ASS10, BS15, BBI+11, CSAdOM17, CH10, LDH+14].  
States [GMBM18, AST+16, ANH+11, BSL+16, DHOG13, EFS16, EK17, EVR18, EP15, FAA15, FD16, GO13, GA12, GTK10, HDHL15a, HDHL15b, HDHL15c, JCGVPT17, KKH19, KT19, KKA+18, KPG18, KB14b, LLBO12, LLW12, LWW12, LGC19, LX11, LS11b, LYSS11, LCK+18, MS10, MN15, MGCC19, MH11, MEH18, PBDW11, RHRC16, SRF+17, SSC+19, SOYC12, SMN+19, SB13, SB15, SSZS16, TN10, Tia12, TSN17, VVV+15, XWSW13, YZGS14b, YK13, YLZ+10, YB11, ZXS+10, ZBB16, ZDT18, dLC17].  
Static [KBC12, BS10a, KZK+12, Lu11, PC14, PNW+16, PM13, WYT17].  
Statistics [Pon10].  
Stationary [BHR15, Can10, Can11, LHMM11, SLT14].  
Stationary-point [BHR15].  
Stationary-wave [Can10, Can11, LHMM11].  
Statistical [JHH+13, PZA15, PTB+15, FL15, GZ14, HYMZ16, 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, DGCI4, GRCL12, JWO15, JS17b, KvdV14, LLG10, LG11, LvG13b, Lvg13a, LL10c, RLDJ17, RS12, SJC11, TCP14].  
Steps [REH13, Zim13].  
Stepwise [DLP11, LZ18, GRCL12, ZL11].  
Stereochemical [WCDM11].  
Stereochemistry [PPJ14].  
Stereochemistry-dependent [PPJ14].  
Stereochemistry-stereodynamics [CSNCS+18, IWD13].  
Steroelectronic [AS11].  
Steroelectroselection [BJS12].  
Steric [RMGB11, MJLW14b, MP17a, YNH+17].  
Sterically [MH17].  
Stern [MBA11].  
Steroelectronic [HLBLCCG15].  
Stevens [BCJC+14].  
Sticks [CVT+11].
stilbene [BW11b]. stk [TBJ18]. Stochastic
[AFPI13, CGP12, AC12, ESD18, KV12, KV13, MS16, MCP18, NC13, PH17, RSLs13, SWB+12, VBD11, ITY+19]. STOCK [BJP15]. stockholder
[FHZA+18], stoichiometric [VI7]. stoichiometry [FSD+18]. Stone
[DWZ+17, YZN13]. stool [FPB12, FB14b, ZCK+16]. storage
[BEM14, BEPM14, DLT17, WKLC12]. Story [Sce07, Sch10]. Strain [DM15, FB12, FC16, FLM11, JWO15, LSL+19, PBE16, She12, SRL+13, VIT+15]. strand [XLY12]. strategies
[AFBR17, BSDP16, cCVG+14, DSX+11, LTT16, Rao11, SC0J13]. strategy
[CLS+10, CZNA11, HJKJ13, KTNN10, KKH18, LLL+10, PHC13, PH17, RVVK13, SRL16, TKNN10, WO15, XHLH16, YDGZ15, SMD18]. StreaMD
[DJS+18]. strength
[Fra15, Fra16, KSC16, LGKS17, MPSG11, YJ17, YHW17]. strengthening
[MS11, LSS11]. strengths [CLK+19, MLC13]. streptavidin
[MLZZ12, ZJZM13]. streptavidin-biotin [MLZZ12]. streptocyanines
[WYT17, XKW18]. stress
[GMBX+16, HXM+16, JMX+16, NIIT15, NFI+16, XFX+16]. stretch
[CK10, RS17b]. stretching [KLS10, KMLS10, TKN19]. string
[BMGF16, JZ17, Zim15]. stringent [DPOS16]. strong
[Kan15, MLZZ12, SDF12, SS19, VVY17, Vik11, ZSLL17]. stronger [KSC16]. Structural
[FHC+19, GLF16, GBL+11, GTT10, GAMAC+14, GWX+12, HS17a, II10, KZK+12, KSD+12, LBTV11, MP19a, NC14, TS11, VSH19, ZWW10, AIGP15, AD10, AKK+16, ALH+10, BBOB16, BPC13, CPV+12, CDS16, CYI+10, DWL11, DH11, GWT+17, GNI18, HS17b, HVS16, KKPT11, KG11, KNE11a, KDT+12, KK13, LLL13a, MCF10, PHC13, PGI15, PNG10, RRR11, RKB+14, RSL16, SFA17, SS13c, TYX+18, VVW+18, WC11, XMSZ16, YV17, ZLW10, ESD18, FAS+18, VPR10]. structurally [TZCK18]. Structure
[BJP15, CBK13, DXL+10, GPK+16, GWJJ12, GBGR16, HLB15, LAHS16, MM19, MHRR11, NC12, NC13, PMG+16, Rab12, SGH+16, VDR14, WZK+13, AFPI13, AR15, AM19, AJR16, AC12, BPPS17, BFH+13, Bds13, CPRS18, CD13, CM13b, Clo15, DKE+17, DKT13, DDP16, DVP14, DGSGVM19, DLW12, EH13, EWK+13, EFD13, FZY+12, FSC+14, GL16, GMSdG15, GRARO+14, GP12, GIK10, GRD+10, GPC16, GBG+19, HASR+12, HNHR13, HS+19, HNYH19, HS14a, HRB+17, HH15, HYMZ16, HZ13, HWL15, Hua16, Ibr17, KTY+17, KKH19, KSM17, KT10, KS12, KKL+13, KLS10, KMLS10, LLBO12, LFB14, LKL10, LHZ+11, LMI+14, LYLX, LPE+10, LGL11, LGI12, LWG12, LLFX16, Mat10, MDT10, Man14, MAP10, MV17, NGAS17, NCT18, OCL11, OLI13, OLA15, PSS14, PdSc18, PML+12, PN13, RL14, RCM+13b, RR11, SHM011, SB10, SM11, SLP+12]. structure [SLIB12, SRS14, SYN+12, SKGB13, SPZP18a, SPZP18b, Tac19, TN12, TTB+11, TG12b, UNT16, VVP12, VHR16, VVBL17, VAA14, VBMA13, VC10, VI17, VLGK+17, WO15, WRM+12, WSG11, YW12, YZZ16, ZRCC11, ZHHX11, CPR18, FDCJ18, OSF12, SA10]. structure-
structure-activity [DXL+10]. Structure-based [CGBK13, DXL+10, DVVP14, GLB16, VKC10, YZZ16]. structured [GEP+14].

Structures [DLT17, SNS16, AHK+19, BHNS14, BPM15, Ber17, CL16, CCOH14, CV12, DVVP14, DH14, DLT18b, DT19, DZA11, GS12, GSS13, HSY+11, HTS17, HPL+18, HS12, Hua16, IYK11, KNE11a, KOY+12, KTO11, KTO13, KDT+12, KSW16, LABSG17, uLhY11, LHZ+10, LLSW14, LüC14, MCA14, MCA15, MCA16, MCA19, MCB10, MCF10, MD10, MC10, MCT10, MCG10, MG15, MCG16, MH11, MH13, MH16, MHN15, MHR11, MBRC16, MO17, Mor15, MIS+15, NHR+10, NH19, NGAS17, NASH15, NC12, NC13, NC14, NS18, NJX+10, NFI+16, OPR16, ORZ11, OSS10, OSH17, OME16, OOK11, PVL+13, PGCT+12, PP10, PGC12, PGS+15, PH12, PG18, PAK17, PPH+14, QLYL10, QZ10b, RSI7a, RAGL11, RA+11, Ray13, RS13, RS14, RVCFF13, RSLML12, RKG11, RSKG14, SN16a, SS+13, SGD10, SJ14, SCM+15, SRF+17, SSC+19, SWM10].

Studies [Ish10, KRTB10, OLY17, RHPWS13, RI10, TS15b].
Kop17a, Kop17b, Kop18, LLH14, LL13a, LYC+13, LWZ+17, MK13b, MAK+14, MB14, MOS12, NW17, OKIS17, OHPR17, OHPR18, PZA15, SRSLO15, SH14, SBC+11, SLG15, SLLL13, SIG+15, TSR+16, WXL+12, WXL17, WBF17, XFX+16, XCLZ19, YPvD13, Yan14, ZLT13, ZKE+17, MK11].


Switching [GA19, AB16b, KOP+14, LCH10]. symmetric [HOM+16, KZK+12, LPS12, RSSG18]. symmetries [GR10b]. Symmetrization [MSK+10, MSK+12]. Symmetrizer [LPS12]. Symmetry [CA10, EP15, VV+15a, BV14, CWZB10, DZA11, Dry14, FF11, HB14, KTT16, KC13b, NDD+10, PZBA13, Sch13, TTN19, VGT16, YKH15, vS18, EB18, XKW18]. symmetry-adapted [FF11, YKH15]. symmetry-invariant [CWZB10]. synchronicity [dSVdM+16]. synthase [AALCM11, EvRC+18, SYH12, XLYZ10]. synthase-catalyzed [XLYZ10]. synthesis [QQY+18, YZL18, ZZWT12]. synthetase [LBS10]. synthetic [SBGP18]. synthons [LZSM19]. syringe [WZ+10]. system [BEEL14, BTT10, BCCO10, CS14, CJSZ10, GRS15, HSY+11, HKNH18, HDM+15, IMSR18, KNK+18, LL11, LYL16, LZY12b, MO18, MLZ12, NTNY15, NS15, RHT+15, SZBM13, TL16, VBDS+11, WLF11, XCLZ19]. Systematic [GP11b, KT18, ML14, SDIP18, SA13, SCMA+17, UT15, VLK+17, AIGP15, BEL+11, FM10, IY18, Ish12, LG11, MAMF19, Pet11, STS15, VLV17, WG12, RFHG10]. Systems [RMM16, AST+16, AKP14, BV14, BGL+18, BVY+12, BK13, BBG+18b, BG13, CCR18, CSS17, CEBO15, CKL+11, CLK11, CAP17, EP12, GG10, Gar12, GP12, GA19, GBW+14, GR10b, GWZX12, HS11, HCD+10, HH18, Hm16, ITIN15, JSX16, JS17b, KV12, KZP+18b, KGM12, KL18, LBGS16, LCPS13, LPLA13, MSC+10, MG14, MOS12, MS12, NYN17, NC10, NLL19, NFG+13, NO16, NNK+16, NS17, ODB18, OPB+12, OC14, PAK17, PAT+10, PBBP11, PD12, QLKI19, RJPB12, RVCFF13, SSO19, SCOJ13, Sch12, Se10, SKGP19, SEJ+18, SH18b, SWB+12, SG13, SMM17, TS16, TCX+13, UT15, WCY+11, WWU12, WS11, YCK16, ZSB+11, ZFS18, ZT14, Hm17, SZL19].

T [BBI+11, CSGOA17, Gil11, MSPC19, MLCD11, OPR16, SRR16, XKW18, YY17, BBG+11, BH13, CGBK13, HLS+13, Sch13]. T-cell [CGBK13]. Table [Ano16-115, Ano16-121, Ano16-122, Ano16-123, Ano16-124, Ano16-125, Ano16-126, Ano16-127, Ano16-128, Ano16-116, Ano16-117, Ano16-118,
Ano16-119, Ano16-120, Sce07, Sch10, AAC+16, Fom11, JMS13, MGS+16. tables [BDdS13, LZ12]. TaBoo [HTS15]. tabu [GBSE11].
TANGO [GKJ+19]. tar [HCD+10]. tar-MD [HCD+10]. target [FMG12]. TargetATPsite [YHH+13]. targets [AFBR17, BK13, MPBJ11]. Task
TD [HL19, TS15b, CCB15, CH10, EFAC13, HRJ+14, HRJ+15, HL19, JRSH14, KKL+13, KP10, LZL+10, LZHH11, LSH+11, LYSS11, RDF+11, SRF+17, SCF+19].
TD-DFT [CCB15, CH10, EFAC13, HRJ+15, HL19, JRSH14, 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
[AM19, 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].
tellurium [RRK16, ZWGO16]. Temperature
[HS17b, KKO+16, LPE+10, LLTC12, PBE16, SY16b, SMM+18, CH16, DKT13, DLSD13, KCK+17, LI11, MK17, MKK+19, OGL10, TLDG+12, TM16, VED10, WMW11, WWTL19, YW12, OCW+15]. Temperature-shuffled
[HS17b]. temperature/Hamiltonian [KCK+17]. temperatures [NMLD13, RHNN10]. tempering [GC18, LAW+16, MO15, MO17, NPTS16, TKT11]. Template
[Mau14, GLF16, KCK+17, ME10, YHH+13]. Template-free [Mau14, YHH+13]. template-restrained [KCK+17]. tension [NPFD13].
tensor [CPZ19, Elk16, EWK+13, GMBX+16, HXM+16, JMX+16, KK17a, NFPD13, NIIT15, NFI+16, TKC+11, XFX+16, YAO18]. tensors
[EPD+11, PHK14]. tepidum [KPG18]. terahertz [KB16]. term [DSF17, JBSQG11]. terminal [IMK+16, YXZZ17]. terminally-
[KLS10, KMLS10]. terminally-blocked [KLS10, KMLS10]. terms [BAS14, CZA11, CWZB10, RRH12]. ternary [RDT14]. tertiary
[OPR16, SM11]. tessellation [MOS12]. Test
[PHC13, BS10b, DPOS16, Wnn18]. tested [HM10]. Testing
[Gill11, IM18, MPSA17, RLD12, JGS+17]. tests
[Ano15-59, CNK97, ENKK+17]. tethered [CZNA11]. tetra [WDLG12].
tetraamines [SB10]. tetracarboxylates [CRC13]. tetracoordinate
[XhD15, ZYW+16, ZLY+16]. tetroalene [ABDGN12]. tetragonal [LKZM18]. Tetrahedral [LBC+19]. tetramer [ish10]. tetramers
[EyL16, SZSZ16]. Tetraoxide [JW12, SLHW09]. tetraprotonated [ZWA+10b]. tetraradical
[CS14, YSSB12]. tetrasaccharide [NP17]. tetraethylvaline [MCF10].
Tetrazine [JW12, MCAG+16, SLHW09]. Tetrazino [JW12, SLHW09]. Tetrazino-Tetrazine-Tetraoxide [JW12, SLHW09]. Tetrel [YKH15].
tetroxide [MCAG+16]. text [HKRS11, HS11]. text-based [HKRS11, HS11]. TF [XMSZ16]. TGMin [CZL19]. Th [MCK17a]. ThCl [LCL+18]. them [ARRC15, Ano11, AM19, BSG18a, CBTZ16, CFC15, CB11a, DLT17, DSM+11, GPM17, HJ13, JMLL13, JHMB+09, JHMB+11, KG15, KNE11a, KRSC12, NYH+17, SBR13, TN12, Tak11, TY10, TS11, VVJ15, VVY17, VVL17, XDL+10, ZYW+10a, GMBM18]. them [WCWV15]. theoretical [CRZ+18, MCC12, ZLW10].

Theoretical [AvKLSP16, 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, KS13b, LCL+10, LWL+11, LLW12, LZY+12a, Lin18, LWXC16, LXFC17, LD18, LJG+11, MLQ+12, MSV16, NFI+16, OSS10, OAN15b, PKK17, PM13, PE11, RS17b, SB10, SMiN+19, SKY+11, STS+10, SZZS16, SLC+17, SGHL13, TDP+12, Tsui19, WMM11, WHDL11, WSL+11, XBSS19, YJN+11, YPC+10, YHG+11, YCGA10, YYT12, YDGZ15, ZYW+10a, ZZL+10b, ZZL+10a, ZYLL12, ZLLL12, ZSZ+14, ZYG+15, ZBMMH15, dSdLB18, BLS10, BAD+19, BE16, CHZ12, CKL+11, CBTZ16, EV14, GG10, HDB15, HGHP14, LWL12, LLD17, LZW+11, LCL+18, MRC+18, MPSG11, MKK+19, NHF+10, NJX+10, PH12, PdSc18, PsPE+10, Pog10, PH10b, RZG+13, RVCFF13, RVP+11, RVCFF13, RVP+11, SSP+13, SSC+19, SD11, SLHW09, SKTT11, SGH+16, Tak11, TL16].

theoretical [UCRL18, WSH10, WZQW10, YK13, YZWC11, YZN13, YB11, Zha12b, dSAdSL13, HDHL15a, HDHL15b, KZK+12, TDP+12].

Theoretically [LLX+19]. theories [OM12, WCWV15]. Theory [CKH19, EVR18, GNC+18, IUK+11, LLX+19, MP19a, SXZ13a, SXZ13b, WM12, AMK11, ALK+15, AR10, Ali18, ARAG17, ABDGN12, AG12, ASS10, BY11, BLCB+13, BZB+13, BG13, CHG+16, CRZ+18, CSAdOM17, CWHH11, CKH17, CCM15, CF14, CC11, DAP+18, DCHL12, FRSA14, FD16, GHL, GZL+12, GQ15, GIY10, GNGCA10, GND+12, GA18, EGEN1, GP12, Han11, HPT17, HII+13, HNN+17, HRJ+14, HRJ+15, HG10, ISN13, IKN13, IM17, JRSH14, JLH+14, JW16, JYS+12, KHBW17, KLN12, KM13, LCW12, LBG16, LCL+10, LLH17, LPM17, MCC11, MMH19, MAK+14, MJH+11, ME10, NPG+18, NMLD13, NO16, Niz13, ORZ11, OZLSB12, PAK17, PML+12, PPH+14, Piel4, Pyy13, QZ10b, QZ10c, QH16, RAGLL11, RJPB12, RCM+13a, RML+15, RB12, RSLML12, RHPWS13, RNS19, Rui11, SM4a, SFG+17, SHL+18, SCW11, SSSM15, SHF11].

therapeutic [AFBR17]. therapy [ZZ12]. there [MLGB16, Sie18]. Thermal [LL10c, ASL+11, BIL10, NGAS17, OZLSBH12, VVW+18]. thermally [FWS+18, IHY15]. thermostabilizing [MLGB16, Sie18]. Thermal [TFQ+11, KSM16, TN12, WD12]. thermochemistry [HDH12]. Thermochromatium [KPG18]. Thermodynamic [LL10c, ASL+11, BIL10, NGAS17, OZLSBH12, VVW+18]. thermally [FWS+18, IHY15]. thermostabilizing [MLGB16, Sie18]. Thermodynamics [DS12a, RS12, BRE16, DMJ17, EHSPT16, HRC13, Kan15, WRM+12, ZYL+12]. thermoelectric [KLZ+18, NGAS17, YW12]. Thermodynamic [EOO+16, NSK18, PAT+10, BE12, BPE16, BB11b, BB11c, CBH14, CC18a, EBPK17b, HDL+17, Hug12, MMB+17, PGY15, PBE16, RNSF+16, RRF11, RKB+14, SS13c, SJC11, SJ16, WC11, dRBO13]. Thermodynamic [EOO+16, NSK18, PAT+10, BE12, BPE16, BB11b, BB11c, CBH14, CC18a, EBPK17b, HDL+17, Hug12, MMB+17, PGY15, PBE16, RNSF+16, RRF11, RKB+14, SS13c, SJC11, SJ16, WC11, dRBO13]. Thermodynamic [EOO+16, NSK18, PAT+10, BE12, BPE16, BB11b, BB11c, CBH14, CC18a, EBPK17b, HDL+17, Hug12, MMB+17, PGY15, PBE16, RNSF+16, RRF11, RKB+14, SS13c, SJC11, SJ16, WC11, dRBO13]. Thermodynamic [EOO+16, NSK18, PAT+10, BE12, BPE16, BB11b, BB11c, CBH14, CC18a, EBPK17b, HDL+17, Hug12, MMB+17, PGY15, PBE16, RNSF+16, RRF11, RKB+14, SS13c, SJC11, SJ16, WC11, dRBO13]. Thermodynamic [EOO+16, NSK18, PAT+10, BE12, BPE16, BB11b, BB11c, CBH14, CC18a, EBPK17b, HDL+17, Hug12, MMB+17, PGY15, PBE16, RNSF+16, RRF11, RKB+14, SS13c, SJC11, SJ16, WC11, dRBO13]. Thermodynamic [EOO+16, NSK18, PAT+10, BE12, BPE16, BB11b, BB11c, CBH14, CC18a, EBPK17b, HDL+17, Hug12, MMB+17, PGY15, PBE16, RNSF+16, RRF11, RKB+14, SS13c, SJC11, SJ16, WC11, dRBO13].
transition-metal [LDZW17].

transitions [AKK+16, BD11, DH11, HS17b, NB18, SPZ18a].

transmembrane [DSF17, LMI+14, LAW+16, WXL+12].

transmission [LLJ12].

transphosphorylation [WXY14].

Transport [DJX+11a, AWF+18, CWHH11, CBTZ16, DMN14, DMN15, DJX+11b, HLWD15, LHO17, LJR+12, NSK18, NS17, PGY15, RJBH18, RSSG18, SLIB12, SY16b, TCX+13, ZYG+15].

transportation [LZY+12a].

trapped [DM15, VIT+15, WLW+10].

treat [CJPTC18].

Treating [JLCA17, SMP17a].

Treatment [HSH15, CSGOA17, GPK12, Has14, HGHP14, MG14, NS10, Sch12, SSWX14, SJL18].

tree [JCPC11].

treecodes [BK13].

trees [AGR11b, RDRC16].

Trends [CXS10, PH15, RLA18, dSdLBNB17].

tri [ZP13].

tri-N-acetyl- [ZP13].

triaxial [YY10].

triangular [TS11].

triangularly [LWZK13].

triangles [She12].

triangularly [LWZK13].

triangulenes [GSMM15].

triarylamine [KGR+16].

triazine [WDLG12].

triazines [YPC+10].

triazol [ZZWT12].

triazole [NS10].

triazoles [GKR13, Ray13, RKG11].

trichlorostannate [PKK17].

tricyclic [VSD10].

Triel [Jab18b, Gra18, YKH15].

triene [ABDGN12].

triethylgermanium [WHX+10].

triflate [SV11].

trifluoroethanol [ARA11b, RDRC16].

Trifluoroethanol/water [JA10].

trifluoroethanol [JA10].

trifluoromethane [CLC11].

trifurcation [LLD17].

trigger [SB18].

triggered [DADGR15, TTC+18].

triggering [AN011, GAV12, GRD+10, HMB+09, JHM+11].

trihalide [Gra18].

trihydride [PM13].

triiodide [VVMY18].

trimer [THP+15, YCGA10].

Trimeric [PMT16, RCM+13a, RML+15].

trimetallic [GLF16].

trimethylsilyl [BIL10].

trinitrotoluene [SH14].

tripeptide [BH15, GMO16, MHO18].

tripeptide-water [MHO18].

triphenyl [AS18].

triphenylamine [MSV16].

triple [ACD+13a, ACD+13b, LOB18, LES19, POB13].

triplet [RS17a, SSC+19, THP+15, ZZL19].

triplets [EK15].

triphosphorylamine [LL10c].

tris [KPL15].

trivial [UK+11].

tRNA [LBS10].

tropocollagen [PP10].

tropolone [DL19].

Trotter [VKAM12].

Trp [EJ13].

Trp-Glu [EJ13].

TRREAT [CM13a].

truncated [CME11].

truncated-CI [CME11].

truncation [ACD+13a, ACD+13b, CS14, IMSR18, MC12].

trust [PLAG11].

trying [BRGN12].

trypanothione [VSD10].

tryptophan [EOA+11, LM18b, PS14, SHB17, VMTL10].

Tsaltis [ZQ10c].

tsscds2018 [RRFV+18].

TTTO [JW12, SLHW09].

tuberculosis [MPNS13].

tuberculosi [MPNS13].

tubular [uLhY11, ZY+16, YLZ+19].

tularensis g [STM+15].

tumor [JAH+17].

tuned [Ali18, BK17b, HZSS17, LCK+18, SZS16].
[CZAF17, MRO17, ER18, SPL+18, DPNM11]. Updated
[SvK18, BCJC+14]. Updates
[AIGP15, Aki16, APK14, AAC+16, BTA+13, BHB12, BCSCJ+13, BSZ+12, Ber17, BJPI15, BFH+13, BBG+18b, CBH14, CSEMB+16, CZAF17, CAT+13, DMIN15, DJD12, DVPI14, DBDP16, DDK14, DWC17, DSK17, ESB13, EWK+13, FN12, FSC+14, GMSdG15, Gar12, GJMAMP+14, GLW13b, GS12, GCP+13, GCC14, GBW+14, GH16b, HLS+13, HRB+17, HDH12, HPT+16b, HPSK12, HHT+13b, HH16b, HG13, HYZM16, HKR+14, HBJ+17, HL14, HC14, IGK16, JHH+13, JJW+14, JLA17, JP15, JCGM18, KS13a, KS15, KK17a, Kan15, KB16, KDR+18, KLJ+17, KJM+17, KDT+12, Kos16, KG13, KWL+16, KK17b, KG15, KYG+15, KAG+12, KSW16, KPF+15, LPS12, LJ+12, LSH12, Lsh15, LrvdSM15, LrvE17, LDB+17, LLZA12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MTD16, MBR+15, MYT18, MSSP17, MB14, MB16, NKJ16, OVI14, OPB+12, OZS+13, OC14]. Updates
[PSS14, PGL+15, PSG+17, PW12, PPM15, PHH+12, PVZ13, PG14, RLLHL12, RNSF+16, Ras17, Rez16, RR14, RdA12, RSR+12, RCM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sic15, SJ17, SWB+12, SDMS13, TNYN16, TSC+13, TTR+12, TNL+12, UU12, VMRS+17, VVV+15b, VAR12, VB113b, WdVN12, WdY13, WPM+15, WF16, Wei12b, WHK+12, WHJH13, WG14, WJC+14, XML+15, XYX17, YWJ+16, YZ16, Yes12, Yes15, YHH+13, ZDKM12, ZLL+13, dVAG16, KKR+13, SR18].


Uroporphyrinogen-III [BEL+11]. Use
[DCOD13, GPM17, HCD+10, MPA12, MMZ14, NPTS16, NC14, NDD+10, QS19, RLD12, WM17, Yes12, BCP+10, CKH19, SJL18]. used
[PGY15, Pie14, PLAG11, TH13]. useful [SMGB11]. usefulness [SP15].

[BS15, Car14, DLL+10, HH10, HPSK12, LLvG10, LG14, MGCC19, MSPC19, MP11, NZM18, QLQ11, SK17, TNG+10, WF16, AASP18, AG11, AS18, ABS+19, AGM+13, AC12, BW11b, BMR11, BDTP11, 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, HNy19, HLW+17, HDL+17, HH17, Höf14, HBL12, HYUS11, HJKJ13, HZSS17, HHWL17, HLEM18, Hug14, HH+17, Ish10, IHJ+13, JLH+14, JMS13, KV13, Kan15, KSO+19, KERY+16, KT10, KLOS10, KGJZ19, KTN10, KP11, LBGS16, LPK16, LRvdSM15, LZ12, LCH10, LCL+10, LMR14, LGH11, LTA+11, LBDP12,
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