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Title word cross-reference

[GT10] [TN12].

[Ben17, KSK11, LGW12, LX11, LWD13, PTK11, Pie14].

[SKMS13].

[RDT14], \frac{1}{2} [RDT14]. \Sigma [LWD13], \Sigma [Kop15b].

[GTK10, LGW12, LWD13, OZLSBH12].

[BHB17, BMFG16, DaadGR15, LPE10, LWXC16, MG11, PGIY10, RRF11, RHT15, TLY12, WRG17, vSGP10].

[CM16].

[GTK10, LGW12].

[CM16], \frac{1}{2} [LSW14, MG11], LHM [BS10c].

[KPL15], (ads) [LLTC12].

[GBGR16, JCG11, LdSRR16, TFQ10, VIT15].

[AS15a, AR10, BE14, BPE16, BP14, CXW14, EB12, EBK13, FD16, Ibr17, JCG10, JLS10, JLH14, KBC12, KKR13, Kop16, KCL14, LZTV10, LW12, LWC16, LWD13, LLB12, LL10c].

[XFX16, YR13, YL11, Yu12a, YZ15b, YXZZ17, ZRCC12, ZRCC11, ZZ10, ZZL10b, ZSW12, ZLL12, ZYG14, ZLY16, dSDdAR10].

[GBGR16, JCG11, LdSRR16, MCK17b].

[MCIK16, SC17].\frac{1}{2} [OPR16].\frac{1}{2} [OPR16].

[DM15, TFQ10, VIT15].

[AS15a, AR10, BE14, BPE16, BLF14, CNH11, BPLL12, BLG10, BKWK10a, BKWK10b, BS10b, BS16b, CK10, CCJ11, CCM15, CKL11, CXS10, DOM11, DLS13, DLW12, DHE12, EP15, EPB17b, FMNC11, GL17, GK10, GWJR18, GY12, GWJJ12, HYL11, HZ11, HSY11, HFSO12, HBL12, HYD10, HRL11, HVS16, Ibr17, JCG10, JLS10, JLH14, KBC12, KKR13, Kop16, KCL14, LZTV10, LW12, LWC16, LWD13, LLB12, LL10c].

[TFQ10], \frac{1}{2} [PMG16].

[TFQ10], \frac{1}{2} [RSKG14, TFQ10].

[TFQ10], \frac{1}{2} [RSKG14].

[TFQ10].

[TFQ10].

[TFQ10].
CKL+11, DLMH12, GZZM16, HSZ+11, KV14, KDS17, MVKS10, MIS+15, OOK11, PM18, RF15, SSGS15, SDF12, YJN+11, Zha11]. π · · · π [CCCLCGRO14], pK_a [BA11]. Ψ [Lü14]. q = 0, ±1, −2 [Xh15X]. r_m^2 [RCM+13b]. → [CK10, Chu10, GTK10, HZ11, HBL12, LWD13, NMLD13]. S_1 [KKL+13]. σ [DPSL16, GZZM16, LZZ+15b, PM18]. σπ [CZY11, YWZ14]. Å³ A’ [MCLD10]. × [SRS14]. v = 0 [LWD13]. x = 1 [CWT+12, LZTV10].

| 1 | ZZWX11, CS17, DLZ15, GTK10, NHH16, SYH12, SRS14, TTB10, UNT16, XLY12, ZsA10. |
| 2 | [DPNM11, MWJ+11, DH17, HOM+16, LGW12, Lüc14, YZGS14b, Yu12b, Yu12a]. |
| 3 | [MWJ+11, 15-crown-5 [MWJ+11], 3-15-crown-5 [MWJ+11], 3-alternate [ZWS+10]. |
| 4 | [YLZ+10, LZTV10]. |
| 5 | ZZWX11, cCVG+14, LL10c, Mor15, Pon10, SOvG12. |

7 [ADF+10, MBR+15]. 7-azaindole [YYT12]. 7-tetraene [ABDGN12].

8 [AAC+16]. 8-formyl-7-hydroxycoumarin [LZHH11]. 8R [BG13].


Ben17, CCLP12, CSGOA17, CRZ+18, DKE+17, GAI13, GBW+14, GWZX12, HRC13, LC17b, LZZ14, MAK+14, ME10, MFR+17, NHHN16, yOTn16, dIRL11, RB13a, RCR+16, RDDS10, RR14, SH15, SS16b, VAMS14, VDVR14, WX5+12, WJG+13, WX12, XSZL11, YOMT14, dVZ17, dSaSL13.

Accurately [Bow16, LFB14, MA16, Zha12b]. ACE [WCDM11, LHL+10].

acetaldehyde [AS11, AAMD11]. acetaldehyde [YZL+15]. acetals [JSW10].


acetylation [FHK+12, IMK+16, LHL+10]. acetylcholine [SRA17].

achim [Spr10]. acid [BLG11, CYY+17, CC18b, CFC15, CM16, CB11d, FD14, FZL+15, Fel10, FP17b, FCE15, GRL+11, GRL+12, HPT16a, HNN+17, HGY15, HCP15, KLS10, KMLS10, LBC+12, LXL+11, LFM12, LP11b, LPMT17, MSLS10, MRO17, NHF+10, OXW16, PHDH13, SISK10, SZBM13, SBW12, SV11, TL16, VMPS17, WC14, WG12, XVN17, ZSB+11, ZWP11, ZHHX11].

acid-catalyzed [CYY+17]. acid-water [TL16]. acid/base [VMPS17].

acid/base [VMPS17]. acidic [APY+16, YDX16]. acidities [ALK+15]. acidity [CRZ+18, CPK12].


Activation [Niz13, AALCM11, DR11, DSM+11, FB12, MRR11, MBFG15, TS15a, WC11, XLYZ10, YXZZ17].

activation-strain [FB12]. activator [BM12].

active [AIGP15, Cas13, DPB+12, LZTV10, PDG+16, SCSW13]. active-space [PDG+16].

actives [EOO+16]. activity [BPC13, DXL+10, GAI13, GHL17, GFPSD17, MJLV14a, RCM+13b, SLY+10, TD10, TTB+11, YB13, ZsA10].

acute [TL+12]. acyclic [ZKH+10]. acyl [PS10].

adcluster [IN13]. Adding [XHLH16, Zha12b]. addition [FWB14, KS13b, NDG14].

Additive [XVA+16, DNS11, HMI+13, TMR+16, VHA+10, VMPS17].

additivity [ZRL+15]. address [LG14]. addressing [cCVG+14]. adducts [LC10, LS11b, ZRCC11].

adenine [BZH14, LLT12]. adenosine [SRA17, WZQW10].

adiabatic [UD12]. adjacency [GZH10]. adjusted [HH15].

Adjustment [BLZ+13]. ADMA [MA17]. AdNDP [KDS17].

adrenergic [CV12, LHIHM16, VKC10]. adsorbate [GBS+17].

adsorbate-induced [GBS+17]. adsorbed [MCF10, PXXW10, SLLL13, SIG+15].

adsorbents [HVS16]. Adsorption [CCJ+11, FVP14, HB15, KD10, LHI1b, PH12, AS15a, BS16b, CMM18, CR14, cCVG+14, Hei10, LL13a, LPP16, LPLS16, LZ14, LT14, LCM+14, NPP13, PGC12, PLZ17, RHNN10, SH14, SDB+16, SKTT11, SYZ+17, VS14,

affinity
[CG15, CZAF17, DLZ15, MCK17a, SSS+13, VL17a, ZJZM13, ZYvIZ14].

After [WZK+13]. Ag
[Rab12, AS15a, IN13, LLTC12, MCF10, PGS+15, SLLL13, YXZZ17].

Ag-nanocluster [AS15a]. against [Gil11, MPNS13]. Ag
[Yan16]. agents
[PsdPE+10]. aggregated [BSL+16]. aggregates [LSH+11, SLP+12, Ber17].

aggregation [RCM+13a, RML+15, WDP+12]. aggregators [RLL+10].

Agonist [HK18]. agonists [CV12]. AgX
[YS13]. AHAS
[SJD14]. aimed
[KS12]. Al
[LCWW10, Pon10, UT15, YR13, GWJJ12, KKR+13, SH14].

Al-hydroxylated [SH14]. Ala
[SZMI13]. alanine
[IO13b, MVKS10, SEM12]. AIB
[MAY15]. alchemical
[BB11b, BB11c, BG12, GMSdG15, GRS15, HLW+17, KB11a]. alcohol
[MS13, ZSZ+14]. alcohol-based
[MS13]. alcohols
[VVY17]. aldehyde
[ZZWT12]. Alder
[CC18a, FB12, FB14a, GNDA+12, LZH16, ORZ11, ST13, dSVdM+16].

Alder-ene
[FB12]. Alderase
[BJS12]. aldol
[HJLV16]. aldosterone
[RVP+11]. algebraic
[GMMP+14, WWD14, YD17].

algebraic-diagrammatic
[YD17]. Algorithm
[WM12, AMGB10, AM10, AYYO17, BW11a, BYE+16, BDdS13, CM13a, CDBM11, CVT+11, CM13b, CB11b, DS15, DJ13, DLSA14, DZA11, FRLN10, GFG11, GPE13, GBD12, HTS15, HEMCZE+14, HQC16, HKR+14, Hug14, Ish10, IJH+13, JCPIC11, KK17a, KNHN16, KN17, KDT+12, LZX16, LZL+13, LZLM16, LZS+17, LLJ12, LTA+11, LMA15, NYN17, NC12, NG10, dRL11, PS17, RMPAM15, Ras17, RSL16, SRSO15, SYH12, SSMW09, SCSW13, SA11, WMW+10, XHLH16, YVEI+17, ZSS+13, vLBBR12].

algorithm-artificial
[WMW+10]. Algorithmic
[LPS12]. Algorithms
[BV14, KGHC15, AGR11a, AC12, CD13, Fom11, GBSE11, KJM+17, Leh15, LLZA12, MS16, MO15, NC14, NOKJ16, RFN15, TRA+16, ZVY+15, dACP12, vLBBR12].

aligned
[KC14]. alignment
[BF15, HRK+10, HKRS11, HS11, MJM+15, RP15, RH11, Ran12].

alignments
[CY10, Ran13]. aliphatic
[CROB16, SB10]. Alkali
[YHC11, Ano11, DDM+15, JHMB+09, JHMB+11, THP+15, ZVY+10a].

alkali-metal
[ZVY+10a]. alkalides
[WXS+12]. Alkaline
[XZ11, Ano11, JHMB+09, JHMB+11, WD10]. alkaline-earth
[WD10]. alkane
[JGS+17, ZST14]. alkanes
[Jo17]. AlkB
[PHC13]. alkynes
[Jo17]. alkenyl
[YZZ+15]. alkyl
[Deu12, RMG11]. alkylthiols
[FVP14]. alkenes
[Jo17, YXZZ17]. All-atom
[SM14b, CS14, DPNM11, HM13, JYC+16, LZZ14, MZZ11, OCW+15, VHA+10]. all-electron
[PGdO+16]. all-organic
[LZZ+15a]. all-siliceous
[Lar11]. allene
[GRCL12]. allenes
[KV15b]. allocation
[NOKJ16]. allophycocyanin
[RML+15]. allostERIC
TSR+16, VVLG17, XZ11, YKO+11, ZSLL17, ZLW10, GFG11, ACD+13a.

approaches [BH13, CME11, DBM+17, ECZWD17, HBI+17, LSH+11, RLDJ17, RR15, VLB+10, YJ11]. Appropriate [LZLC13]. Approximate [Gav12, KV12, KV13, RP15, RZ16, SM14a, HH16a].

approximation [AO10, Boz18, Cas13, HH17, Shc12, WHM10, YD17, YN15].

approximations [CGPP11, HAGK10, MKH+13]. April [Ano12u]. Appropriate [LZLC13]. Approximate [Gav12, KV12, KV13, RP15, RZ16, SM14a, HH16a].

approximations [AO10, Boz18, Cas13, HH17, Shc12, WHM10, YD17, YN15].

arbitrary CHC+13, EPD+11, GP12, HAL14]. archetypical [vSGP10]. architectures [MJBM12, OB+12, SOM+13]. area [FZY+12, GY10, HWLW11, KRSC12, KTSW11, MOS12, NW17, WXL+12, WBF17, dCLFGL13]. areas [MK13a, ZKE+17].

armchair [LPLS16, RRK14]. aromatic [HC16, AH10, FVB10, JHB+13, Kar17, KDS17, MVKS10, PRJ+17, PL18, SSA+17, TTR+12, TDKT10, WSZW15, YCK16, YHC11].


aromatic [HC16, AH10, FVB10, JHB+13, Kar17, KDS17, MVKS10, PRJ+17, PL18, SSA+17, TTR+12, TDKT10, WSZW15, YCK16, YHC11].


assemblings [CBTZ16]. assembly [AGR11b, Hei10, JM11, KL16, uLhY11, Mau14, OAN15b]. assess [SJ16].

[DLSA14, HAL14, NDG14, QLYL10, WCDM11]. Asynchronous
[XFG+16, XFG+15]. Aten [You10]. atmospheric [BCNH+11]. atom
[BS10b, CVT+11, CS14, DPNM11, DM15, FSC+14, GBVA11, HRK+10,
HM13, JYC+16, JGS+17, Jor17, KV14, LC10, LZZ14, MZZ11, Niz13,
OCW+15, ST11, SM14b, SYH12, Tsi17, VIT+15, VHA+10, VKAM12, VI17,
VDVR14, YPKB12, YHCS11, dLC17, dVZ17, YMP14]. atom-aromatic
[YHCS11]. atom-based [dVZ17]. atom-centered [VI17]. atom-typing
[YPKB12]. Atomic
[BMFG16, EPD+10, KGM12, AYYO17, BLDK+13, BB11a, CP15, EKH14,
Elk16, EP12, EV14, HS12, JMLL13, JXSW15, KOP+14, KR12, Lar11, LZGS11,
MK13a, MPA10, MPA12, Mat10, MPBJ11, NOKJ16, OBW12, OV14,
Pol13, RB13a, SS16b, SE14, SMP17b, SFCCK+14, SFCCK+15,
STS15, TY10, VGV+11, Vybi5, Vybi6, YWZ14, YKH15, ZYW+16].
atomic-resolution [BMFG16, NPG17]. Atomistic
[BH13, CHKR10, MBA14, SE14, BLKP12, CZNA11, DDP16, HDPM14,
LZ12, MSC+10, MMZW14, RO14b, RSG+10, ZST15]. atoms
[ARAG17, ARLP13, BSF18, BSPP+13, DC13, EV14, GAMAC+14, HSB+11,
HGCCGR+16, IN13, LHSH12, MP17a, Pyy13, SFCCK+14, SFCCK+15,
STS15, TY10, VGV+11, VHG+11, YHG+11, 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, THP+15]. attack [MY+13]. attenuation [SPH11]. attract
[VYV18, CZAF17]. Attracting [ZSB+16, VYV18]. Attractive
[MKH+13, IO13a, SNDK16]. attractive/repulsive [SNDK16]. attributed
[CM16]. aufbau [EKH14]. augmented [BVHI17]. austenitic [vADC+14].
auto [LDH+14]. auto-encoder [LDH+14]. autocorrelation [LL13a].
AutoDock [TO10]. Autodock4 [CSSB11]. Automated
[BW15, EMD17, GMsG15, OZS+13, PBG17, SM11, Zim13, CCLP12, KG13,
LLHM16, MN15, NKJ16, SH18, FN12, JBAM11, JSD+11]. Automatic
[AJR16, Leh15, UKS11, KSH+17]. automating [IGK16]. automaton
[Li14a, Li14b, YS13]. Auxiliary [Hil13, TKN13, HDL+17]. availability
[HJ13]. available [SPR+13]. averaged [HCD+10, WLO+17]. averaging
[DB12]. Avoiding [BB11a, dACP12]. axial [SNDK16]. axis [KGM12]. Aza
[NDG14]. azaborine [EFB16]. azaborinine [RS17a]. azacrown
[ZGW+10a]. azaindole [YYT12]. azetidine [SHL+13]. azido [WDLG12].
azidolysis [BCP+10]. azulene [WWKS16]. azurin [SOvG12].

B [MLQ+12, UT15, YLZ+10, BWKW10a, GTZ+18, HJ13, HQC16, LLLM11,
BACE [CS17]. BACE-1 [CS17]. BACE1 [ETLS17]. Bacillus [CPK12].
back [GWT+17, REH13]. backbone [AB10, CKP10, CHP11, FZY+12,
Benchmark [WSZW15, AF14, ANH+11, CSXZ17, cCVG+14, GAI14, KG15, RS13, ZWGO16, IKN13]. benchmarked [XYW+14].

Benchmarking [Ben17, GAJ+17, Hug12, LCM+14, GP11b, HRJ+14, HRJ+15, HZ13, JRSHP14, KSM17, RSG14]. benchmarkings [GPdC+16].

benchmarks [ZDKM12]. bending [KB11c, Sch13]. Bennett

[BB11b, KB11c, dRBO13]. benzaldehyde [Lu11].


Beta [KRSC12, HLH+12, Hug12, LH11, LJR+12, SKKS13]. beta-barrel [LJR+12].


[AF14, BM12, KDS17, yOaCG10, XHLH16]. between [ALW+10, ASL+11, AR10, ACS12, BSF18, CCCLR014, CC18b, CZH12, CQFC10, COOH14, CB11a, dRCFGRB18, DHP+11, Den12, FD14, FC16, GYS+10, GO13, Gav12, GKS14, HvM16, HvM17, HWWL17, KTT16, KWWB17, LDA+10, LLL+11, LW11, LYL16, LWL+16, LvG13b, Luc14, MS17, MSSH17, OHNK11, OCL11, PRJ+17, PL14, RSHR15, SBW12, TTR+12, TSN16, WCT+11, WFZ+18, Wei12b, YHG+11, YKH15, YDGZ15, ZY14, ZBMZH15]. Beyond

[PNW+16, SCOJ15]. BH [LVTV11, LBTV12, Kop15b]. Bi

[RDT14, DM15, VIT+15]. bias [KEPM17, KS12]. biased [BG17]. biasing

[MJC14, OZ14]. bibliography [Pyy13]. bicarbonate [VPR10]. BiCu

[LLL11]. bicyclically [Alig17]. bifunctional [BEM14, BEPM14]. big

[MPA12]. big-bang [MPA12]. Bilayer

[vRWS17, II18, KLN16, RBOH11, SLX+10, WHAS+10, WHAS+16]. bilayers [BPPS17, GBL+11, PVMI0, PS10, RI10, TG12a]. Bimetallic [GEP+14, DAdGR15, GTT10, KKPT11]. bimolecular [CSADOM17].

binary [Hua16, LAS+14]. Binding

[FPB12, GR515, HXS15, JKDB12, SSP+13, ZP13, AALCM11, ALW+10, ABD11, AS10, AC11a, ACS12, BHNS14, BTMS13, BVHI17, BEL+11, CBP+15, CDM13, CLA16, CIKT13, CZY11, CS17, CAF17, CHR+12a, CHR+12a, CPK12, DHP+11, DS12b, DVVP14, DAB16, DPOS16, ETL17, GHK12, GDV17, GWZ15, GEP+14, GPdC+16, GAY+17, HDK+12, HYZZ13, HPL13, HNW07, HNW12, HGI13, HWWL17, ISP+10, JCP14, JZ12, KZW+16, KTO11, KTO13, KDT+12, Lar12, LL10b, L.JW11a, LW11, LCA17, LBS10, MLZ12, MGWR12, MSK12, MFR+17, MNNK10a, NST14, NHI16, NWI17, NFG+13, NF17, NN16, NO16, NKK+16, OBW12, Oht16, OHNK11, ORS16, OCLM14, OOT15, PGC+12, PBLdS12, PSG+15, Pla11, RLDJ17, RCR+16, RDDS10, RAR+11, RO14b, RZ16, RF15, SPS+12, SRA17, SOD+11,
STM⁺¹⁵, TYZ⁺¹⁶, TS¹⁵a, UNT¹⁶, VVG¹³, Vor¹⁰, VM¹¹, WS¹⁰, WNP⁺¹⁶].


BION [PZA¹⁵]. bioorganometallic [SDL¹⁴]. biophysical [FN¹², Mat¹⁴, RTP⁺¹³]. biophysics [HRHI¹⁷]. biosynthesis [BEL⁺¹¹].

bonding-induced [YLZ+10]. bonding/back [PKK17]. bonding/back-bonding [PKK17]. 

Bonds [WFZ+18, DGB+13, ED15, FPR14, Gra18, HH15, Jab14, JJJ16, LHZ+11, LZL+15b, LZY12b, LDG+15, OOK11, Rob13, SM16a, SK13, SJ16, YLL11, YKH15, YJ17, ZLY+16]. 

BonnMag [BBG+18]. Book [Sch10, Spr10]. boost [KV15a]. borafluorenes [ZQ14]. 

borane [BEPM14, Kop15b, LC10, SJZ+15]. borane-cyclic [LC10]. borates [GWJJ12]. 

border [SK12, SK17]. borides [ZWMW10]. born [AB16b, BLZ+13, DSF17, FCE15, HWLW11, KCPMG12, LL10a, LCH10, PS13, RSB+13, SZTSM10, SSBW14, VMPS17, WWKS11]. 

boron [BEPM14, Gra18, GAMAC+14, LT14, Oht16, PGC12, VS14]. boron-doped [VS14]. 

boron-nitride [LT14]. boryl [LC10]. 

BOSS [VKTRJ15]. BOSS-Gaussian [VKTRJ15]. Bosutinib [GMASBF16]. 

both [AST+16, FNSF+11, LX11, THI3]. bottleneck [SRR16]. bound [FLM11, GPK+16, LFM12, MAK+14, PMG+16, PZA15, XWSW13]. 

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


[APK14]. builder [KOY+12, GS12, WCJ+14]. Building 

[MB14, CBP14, GS12, KSW16, MJBM12, RLG14, Tak11, TJB12, VVY17]. building-up [Tak11]. buildu [SS13a]. built [FCPM14, KOP+14]. bulk 


butane-like [WKC11]. butanol [BS10b]. Butene 

WCY+11, WWKS16, YZZ+17, ZYG+14, ZLY+16, BS16a, VAMS14, Ben17, BWKW10a, BS16b, BH13, CG12, ED15, FL15, GWT+17, GMSV14, GZZ12, HJ13, HV16, IMK+16, JLS+10, KV14, KP10, LFB14, LLC17, LDH+14, MSV16, MH11, Niz13, OPR16, PTK11, Pie14, PZBA13, RWR+13, SNKD16, TFO+10, TFO+11, TS15a, VAR12, VED10, WKC10a, WLW+10, WS10, WL14, WTH+16, WS10, YDZ15].

C-terminal [IMK+16].

C2 [KYCL11].

C2-methylation [KYCL11].

C60 [SBW12].

c7rfjv [Ano15-59].

Ca [BHB+17, HBI+17, LZTV10, LPE+10, LBTV12].

CABS [LK11].

CABS-NMR [LK11].

Caffeine [FF11].

Cage [GLZ17, LZ14, OAN15b, WLW+10, WCY+11].

cage-like [OAN15b].

Caging [DPB+12].

Calbindin [PNG10].

Calcium [BHB+17, HBI+17, LZ14, OAN15b, WLW+10, WCY+11].

Calcium-induced [PD12].

Calculate [GH16b, BCSCJ+13, BACSCJ+10, HDK+12, PSC11, SK17, Yap11].

Calculated [CHP11, GY10, KJDB12, MJKV14a, MRK11, NMLD13, SKMS13, Yan11].

Calculating [PNI13, SK12, WNP+16, WWD14, CPK12, EFS16, EPD+11, HAI+16, OK16, SM16a, WYT17, dRBO13].

Calculation [Fer13b, Fer13a, KSH13, MY17a, MMJ10, MS15, SH11b, SOD+11, SOvG12, AC11a, Bac12, BW11a, BK17b, BD11, BL12, CPR18, CHG+16, CG15, CX10, DKE+17, DXX+11, FD14, GM11, GREA11, GCW16, Han11, JIS13, KNH16, KN17, KB16, KDB13, LFN+10, LLW12, LZW+11, MYT+14, MLC13, MS12, NNY17, NFDP13, PDM10, PAK15, Pie14, PW12, RO14b, RZ16, RB12, RRK16, SBV10, SLIB12, SCSW13, SACdG14, SMM17, SR11, SRL11, UTL12, VV+15a, VV13, WDHZ13, ZZ14, ZZL+10b, ZLLL12, HH10].

Calculations [HBI+17, AR10, AAC+16, BE12, BLL13, BS10a, BTMS12, BH15, Bou14, BGI2, BLZ+13, CR14, CCJC10, CS17, CKKK16, CMB10, CXX10, CHK10, DHG+11, EFAC13, EK17, EKW+13, EP12, EB12, EBK13, FA15, FE14, GRARO+14, GMO16, HASR+12, HYL+11, HS14a, HB14, HSH15, He13, HG10, HG13, HBL12, HYS11, Ibr17, IMS18, JCG+11, KKK17a, KB10, KKN11, KGH12, KKR+13, KERY+16, KCPMG12, KKL+13, KSH+17, LEQ13, LM11a, LCH10, LYES+13, LCA17, LzG12, LCM+14, Lun12, MK17, MCD10, MCK17a, MCR17b, NW17, NN18, ONH11, OLA15, OOT15, OZLS12, PBL12, PTK11, PH14, POB13, PBBP11, PDG+16, P131, PGW+17, RAR+11, RHT+15, RLD12, RR11, REV+17, R10, RK15, SH15, SRS10, SP13, SS16b, SCW11, SWR11, SRS14, SMP17b, SDMS13, SHB17, SK17, STT1, TLG+12].

calculations [TS10a, UHH+11, VLB+10, VKAM12, VKNT16, VHR16, VFR16, VMM17, VI17, WC13, WSW15, WHK+12, WTH+16, WXY14, XY+14, YW+16, YD17, YN15, ZRCC11, ZLT13, ZLT14, ZWMW10, ZH12].

calculator [dCLFL13].

calibrate [VVLG17].

Calibration [CBP14, DDM+15].

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

Call [ZPF14].

Can [ASMS10, IMS18, KV15b, LZW+11, PLAG11, SHL+13,
CIKT13, LCB10, TCPPC14, Zha12b. CANADA [Fel10]. cancer
[CPN+17, RHNN10, BW11a, HRK+10, KCK+17, PHH+12]. CaO [BL12].
CAP [EFS16]. CAP/SAC [EFS16]. CAP/SAC-CI [EFS16]. capabilities
[AAC+16]. capability [LC10]. capacity
[KOP+14, PGC12, WKC10a, WKLC12]. capillary [NFPD13]. capture
(GLZ17). Car [KCK+15]. CARB1/TIP3P [SA10]. carbozole
[JYS+12, SLC+17, YJN+11]. carbazole-based [SLC+17].
carbozole-fluorene [YJN+11]. CarbBuilder [KSW16]. carbene
[CWT+12, LXZ+10, TCPPC14, WS11, WS12, dSDdBNB17]. carbenes
[BSDP16, KYKR15, RF15]. carbocation [ONTTL16]. carbocations
[OPR16]. Carbohydrate [ZYvIZ14, NMF+14]. Carbohydrate-binding
[ZYvIZ14]. carbohydrates [CP15, HH11, JSD+11, PLH16].
carbon [SC17, AS15a, ASL+11, BPE16, CME11, DI11, Den12, DC13, FTR15,
GSM15, GPK+16, GBS+17, GZZ12, JWO15, KGHK12, KV14, LPLS16,
LL10c, LT14, LK16b, OCW+15, RHNN10, RRRK16, VS14, WYL+15,
WDZN16, YZN13, YZZ+17, ZYW+16, ZWF15]. carbon-beryllium
carbon dioxide [Sea10]. carbonic [SSP+13]. carbons
[MKB+13, RVB+12]. carboxylate [DQ16]. carboxylates [AARP17].
carboxylic [LPMT17, RB12]. card [SR11]. Carlo
[LHMM11, Aou16, DNN15, BFH+13, CLK11, CG12, CTP13, CAP17, FFA14,
GP12, GPM17, HFSO12, HMM10, HYUS11, HQC16, HHHY10, IH+13,
LPK16, LMZ11a, LZ12, MS16, MBRC16, MOS12, NDW15, OPBR17, PSS14,
PS13, Pn10, PHH+12, RHNN10, RdA12, SCOJ13, SAGC16, SMRM+17,
SE14, UU12, ZLM+15, ZW17]. Carlo/Brownian [DMN15]. Carlo/molecular
[RdA12]. carotenoids [PVAM16]. carrabiose [YSRSS10].
carrier [SFDE16]. carriers [GMASBF16]. Cartesian
[REH13, FHMB15, Elk16]. caryolene [ONTTL16]. caryolene-forming
[ONTTL16]. CAS [MH11]. cascade [HS17b, ONTTL16, ZZWT12].
cascaded [HLZ+15a]. case [Alg17, ASMS10, BM12, BG13, CCLP12, CB11c,
DOM+11, DS12a, EFOD13, EQA+11, GH10, GKR13, GPdC+16, HSH15,
KB13, LPAS11, LP11a, LT13, MIS+15, OME16, PVAM16, Ray13, Rod13,
RG11, RCM+13b, RJS17, SRF+11, TLA10, VKNT16, ZTH+15, ZAR+11].
cases [GREA11]. CASPT2 [SGWA17, VFRAR16]. Cassandra [SMRM+17].
CASSCF [KKL+13, LGZ15, SGWA17]. CASSCF/CASPT2 [LGZ15].
CASSCF/MC [KKL+13]. CASSCF/MC-XQDPT2 [KKL+13]. CAST
[GBW+14]. catalysis [Can10, Can11, LHMM11, MG14]. catalyst
[BEM14, LLC17, YZ15b, ZSWL12, dSDdAR10]. catalysts
[BEPM14, JAB16, NJX+10, WJX+10]. catalytic [GHL17, KV15b,
ONTTL16, SJD14, SYL+10, SOY12, UKS11, WZQW10, dSDdAR10].
catalyzed [AS11, CYY+17, CCJC10, CPL11, HPT16a, HDB15, HJLV16,
KB13, KT12, MG15, QLYL10, TLA10, Tsi17, VCM15, WCWW11, WXY14,
catastrophe [ABDGN12, GNDA+12]. catechol [PBLdS12].
catechol-O-methyltransferase [PBLdS12]. Catenanes [LAHS16].
cathepsin [ETLS17]. cation [CCCLCGRO14, CGPP11, DLMH12, DDM+15, RMGB11, SSGS15, ZYL+12].
Cationic [HIJ13, WJX+10]. cations [CC18b, CGPP11, DLMH12, DDM+15, RMGB11, SSGS15, ZYL+12].
cations [CC18b, KGR+16, LCL+10, LdSRR16, PVS12, SBD+17, Tac17, THP+15, ZYW+10a, ZWS+10].
cations [CG18b, KGR+16, LCL+10, LdSRR16, PVS12, SBD+17, Tac17, THP+15, ZYW+10a, ZWS+10].
cations [CG18b, KGR+16, LCL+10, LdSRR16, PVS12, SBD+17, Tac17, THP+15, ZYW+10a, ZWS+10].
cations/nucleobases [CC18b].
cavitand [CC18a]. cavities [HRB+17, ZSB+16]. cavities/vacancies [HRB+17].
cavity [ZWS+10]. CAVS [SDZ17]. CB [BTMS12, CC18a, ILKR11]. CBS [KG15]. CBS-QB3 [KG15].
CC [Gil11, LLTC12]. CC2 [SGWA17]. CC3 [LZ14]. ccCA [RJWW12].
CCSD [BBI+11, CSGOA17, Gil11, KK17a, KKL+13, MVKS10, OPR16, PC14, RS13, SRR16, SB14, YJ17].
Cd [SLIB12]. CDOCKER [GLB16]. C == [CROB16]. Cefotaxime [MFM+12].
cell [ACS12, CGBK13, Elk16, Fon11, Gon12, JMS14, SRL+15, VAA14, dACP12].
Cells [FPV13, ACS12, DZA11, DGL+13, JYS+12, LZL+15a, SV11, SLC+17, TZ12, YJN+11].
cellular [VBD11]. cellulose [GS12, LHT15].
Cellulose-Builder [GS12]. cementite [VED10]. cementite-type [VED10].
cementitious [TZ11]. CENCALC [SDMS13]. census [PPUBGD10].
centric [LABSG17]. CEPA [Sch12, SB14]. ceramics [RKB+14]. CERES [CPRS18].
Cerium [SRL+15]. CF [JCG+10, NMLD13, RVdB16, ZLLL12, AR10, CROB16, NMLD13, ZLL+10a].
CFCF [NMLD13]. CFCF [JCG+10]. CH [AR10, LWD13, LG+11, OZLSBH12, TLdG+12, WLZ12, ZLL+10b, ZYLL12, ZLLL12, BS16b, CK10, CXW14, KY12, HV16, JCG+10, KBC12, LW12, LGW12, LLTC12, LG+11, MC15, OOK11, RVCFF13, TCPPC14, VY17, VDV14, WHX12, ZLL+10a, DR11].
CH/ [OOK11].
Chaff [NM+14]. Chain [rRGWS17, BFH+13, CHK10, HAL14, KV14, KLS+10, KML10, LPS+13, LZG11, LP11b, LGl13a, LLLM16, OZ14, PD12, PS10, QZM11, SA13, SIS10, SZB13, TSN16]. chains [AF5W16, FP17a, JSW10, LZZ14, NPP13, Pla11, PLH16, TLdG+12, TS15b].
chalcogenides [SPS+12]. chalcone [CPL11, YZ17]. challenge [SDM+16].
Challenges [HGY15, KHGB17, HLvV13]. challenging [CAP17, VT14, WLF11]. change [EMD17]. changes [GDV17, GBS+17, HB15, LK13, MLV14b, MO17, RO14b, YZGS14b].
Changing [XVN17, LLvG10]. channel [HYZY13, PV+13, SFB17, SY16b, TCX+13]. channels [KC13a, LL10c, OKIS17]. character [BMB13, Cas14, Ibr17, RIJ+11, YSS12]. characteristics [DPSL16, Gav12, LT14, Mat14, RDT14, TZ11]. Characterization [VT14, XWSW13, CBP+15, DGL+13, GBW+14, GZZ12, Kop15b, MJBM12, MPA10, RNP13, ZYG+14]. Characterizing [LH11, PRSG13, She12, Yu12b].
characters [LSH$^{+11}$, ZLL$^{+10}$]. Charge
[CMF$^{+17}$, JM11, RDT14, SFDE16, AS15b, ANH$^{+11}$, ALH$^{+10}$, BCSCJ$^{+13}$, BE16, CS14, CBTZ16, CMS13, Cor17, DS12a, DWR17, DAdGr15, EFAC13, ENKK$^{+17}$, GMG$^{+10}$, HLWD15, JCGVPHT17, JZMJ14, Kan15, KVR10, LLLM11, LPE$^{+10}$, LBPD12, MSV16, MHRR11, MPBJ11, NN18, OBW12, PL14, PTB$^{+15}$, RO14b, Rice16, REL17, SPS$^{+12}$, SSGS15, SMP17a, SFLG$^{+17}$, SLC$^{+17}$, TN10, TKNN10, UT15, VPR10, VAR12, VL17b, WCT$^{+11}$, WWCL15, YK0$^{+11}$, YWZ14, YLZ$^{+10}$, YJ17, ZDZM13, dLC17]. charge-assisted [SSGS15]. charge-inverted [UT15, YJ17]. Charge-transfer [JM11, ANH$^{+11}$, EFAC13, YLZ$^{+10}$]. charge-transport [HLWD15]. charged [BK13, KD10, MRO17, NPP13, RJS17, Tsi14]. Charges [WFZ$^{+18}$, CCB15, IM17, JMLL13, RB13a, SN15, TBSM12, VSA11, Yan14, ZBG11]. Charles [HIS17]. CHARMM [MSK$^{+12}$, AKMY18, BF17, DPNM11, GLB16, GZM11, HBJ$^{+17}$, HC14, JCl$^{+17}$, KLJ$^{+17}$, KYB13, LZdIL$^{+10}$, MSK$^{+10}$, MMZW14, RR14, VHA$^{+10}$, WCJ$^{+14}$, XVA$^{+16}$, YHVM12]. CHARMM-based [MMZW14]. CHARMM-compatible [KYB13]. CHARMM-GUI [HBJ$^{+17}$, KLJ$^{+17}$]. CHARMM27 [ST11]. CHARMM36 [HM13]. CHARMMing [WPM$^{+15}$]. Chatt [Bac12]. CHCICH [WLHZ12]. CHEM [ABB$^{+13}$, CHR$^{+12}$b, HNWF12, HLXH18, ICS$^{+13}$, Kne11b, MSK$^{+12}$, RK16a, SFCCK$^{+15}$, SMM15a, GCC14, GKV$^{+13}$]. Chemical [BLG10, BCP$^{+10}$, JCGVPHT17, OM12, SLLL13, VGTL16, ALK$^{+15}$, ASS$^{+17}$, AAC$^{+16}$, APA$^{+14}$, Bac12, Ben17, Bou14, Cam15, CHP11, DKE$^{+17}$, DS12a, DI11, DB12, EOQ$^{+11}$, FB10, FVB10, GH10, GGM$^{+12}$, GPBSM11, GPBSM12, HPT$^{+16}$b, HHDC16, HJ13, Ihl12, JKS$^{+16}$, KV12, KASH14, KP11, KL11, LHZ$^{+11}$, Li14a, Li14b, MDTD13, MDTD16, MN15, MAPB10, MSV12, MSSP17, MFR$^{+11}$, MMJ10, MH10, NCV10, NC13, NC14, OKIS17, OSIG17, ONTT16, OC14, PTK11, PGDo$^{+16}$, Pie14, PBG17, RK15, RSKG14, SRA17, SLT14, SCOJ13, SEF$^{+16}$, SKMS13, SHB17, TLA10, TG12b, TR12, UD12, VBMA13, WBT10, WCT$^{+11}$, WF16, Wei12b, WL14, Wu10, WDP$^{+12}$, YZ15a, YB16, ZY14, ZBB16, ZT14, dCDP15, VBD11, Chua10]. chemical-bonding [MDTD13]. Chemically [EFAC13, ZZ12, Zin13]. chemist [DHE$^{+12}$]. chemistries [BS10b]. Chemistry [Ano10b, Ano15-59, HJG09, Spr10, All11, BRP$^{+12}$, BGR13, CBH14, DDM$^{+15}$, FML11, GHV17, IGK16, JBB$^{+11}$, KTN10, LK16a, OZLSBH12, PWN$^{+16}$, PPUBG10, RZG$^{+13}$, Rez16, REL$^{+14}$, TKNN10, TF15, VVP12, VV14, WDY13, ZYV$^{+15}$, GS16, MFEM16, XFG$^{+16}$]. ChemNetworks [OC14]. chemosensing [LZIH11]. chemosensor [LZL$^{+10}$]. ChemY [Pet11]. CHFCF [NMLD13]. chi [EJ13]. chignolin [HTS15]. chiral [LG14, PC14, ZPP$^{+16}$]. chirality [AS15a, DZA11, PBBP11]. chirality-based [PBBP11]. Chloride [KJ10, KLN16, Rab12, SG10b]. chlorides [RRF11, YZGS14b]. chlorine [Sani17, ZBMZH15]. chloroform
SOM$^{+}$13, SJ17, SM15, SAvG15, WBF17]. Coarse-grained
[MSLS10, NST14, BLKP12, CAD16, HHWL17, JC16, KCK$^{+}$17, KVQC$^{+}$11, KL10, KMLS10, LZ12, LZX16, LZZ14, LZLMP16, MBC11, MBC13, RSG$^{+}$10, SLX$^{+}$15, SDZ17, SJ17, SM15, SAvG15]. coarse-graining
[BJP15, GMPB12]. cobalamin [AALCM11]. cobalamin-dependent
[AALCM11]. Code [REL$^{+}$14, BTT10, CPRS18, GHK12, GP12, LLH14, LCPS13, RJR14, WKC$^{+}$10b, vW11]. codes [KSH$^{+}$17, RKGN10]. coding
[MSLS10, NST14, BLKP12, CAD16, HHWL17, JC16, KCK$^{+}$17, KVQC$^{+}$11, KLS10, KMLS10, LZ12, LZX16, LZZ14, LZLMP16, MBC11, MBC13, RSG$^{+}$10, SLX$^{+}$15, SDZ17, SJ17, SM15, SAvG15].
}[SOM$^{+}$13, SJ17, SM15, SAvG15, WBF17]. Coarse-grained
[MSLS10, NST14, BLKP12, CAD16, HHWL17, JC16, KCK$^{+}$17, KVQC$^{+}$11, KL10, KMLS10, LZ12, LZX16, LZZ14, LZLMP16, MBC11, MBC13, RSG$^{+}$10, SLX$^{+}$15, SDZ17, SJ17, SM15, SAvG15]. coarse-graining
[BJP15, GMPB12]. cobalamin [AALCM11]. cobalamin-dependent
[AALCM11]. Code [REL$^{+}$14, BTT10, CPRS18, GHK12, GP12, LLH14, LCPS13, RJR14, WKC$^{+}$10b, vW11]. codes [KSH$^{+}$17, RKGN10]. coding
[MSLS10, NST14, BLKP12, CAD16, HHWL17, JC16, KCK$^{+}$17, KVQC$^{+}$11, KLS10, KMLS10, LZ12, LZX16, LZZ14, LZLMP16, MBC11, MBC13, RSG$^{+}$10, SLX$^{+}$15, SDZ17, SJ17, SM15, SAvG15].
}
[ZSL+11, GMBX+16, RLDJ17]. compilation [NKJ16]. complementarity [GPS10, OAN15b]. Complete
[SN16b, CSKH15, LYZ+13, OAN15a, SPS+12, SCSW13, TCB16]. completeness [Leh15]. completeness-optimization [Leh15]. Complex
[DLT17, HBL12, ANH+11, BLF14, DaDGr15, Dry14, FFA14, GCWS15, HB|+17, Ishi10, KBC12, KGHC15, KSW16, LLL+11, LZZ+11, LLI1, LWWC16, MLGB16, MY17a, MY17b, NCV10, OME16, OC14, PPUBGD10, QLYL10, SLT+15, SKK13, SL17, SYH+12, TDP+12, WKLC12, WCCW11, WHX+10, ZT14]. complextation [CBP+15, SNS16]. Complexes
[EHSP16, GpdC+16, SKGB13, AvKSP16, AMK11, ASMS10, AK10, BcSC1+13, BLFZ13, BLDK+13, CSGOA17, CPRS18, CWT+12, CMD13, CZH12, CGPP11, CAT+13, CMS13, CM16, CB11d, DS12b, DLP11, EPH+13, ED15, FHW+11, FCE15, FPB12, FB14b, GK15a, GHL17, GPK+16, Gil11, Gra18, HDK+12, HSV+11, HKR12, HLB15, HRJ+14, HGH14, HRJ+15, HDP14, HG10, JRSHP14, KT12, KPL13, KTK17, LS11a, LLC+10, LWL+11, LHWW14, LZZ+15b, LDZW17, LXZ+10, LYSS11, LZZ+11, MC10, MFR+11, OSHG17, OOT15, PGCT+12, PHK14, PM13, PZBA13, RRH12, RHPWS13, RLD12, SB10, SLB12, SPR+13, SDL14, SGH+16, TLY+12, TS15a, Tru18, TS10b, VLB+10, VV17, WL14, XMSZ16, YKH15, ZCK+16, ZRC12, ZZL+12, ZLZ14, ZDX11, ZYW+10b, ZYW+10a, ZBMZH15, vSGP10]. complexity [GP12, NSP15]. component
[CLA16, CSKH16, DMJ17, HKR+14, JKS+16, KMI3, NASH15, PSP15, PW12, RK15, SV11]. components
[CHR+12b, CHR+12a, MBT14, Pil17, XTG+11]. composed [ZYL+12]. composite [KG15, SLG15, TNSS17]. composites [AS15a]. Composition
[PBLdS12, SB13, AO10, FCL+10, GMSV14, GJMPAM+14, HDL+14, HAP+12, NKN+16, SM14a, XSSZ11]. Computational
[Alg17, Anol10b, Anoi5-59, DPB+12, ED15, ECZWD17, EOA+11, GSI16, HYYZ13, HJG09, Hei10, HRL11, JS17a, JLS+10, KAR12, LBS10, Lu11, MFM+12, MFEM16, MSAK12, PGCT+12, SGM+13, TKXT13, XFG+16, XLYZ10, YHK+10, ZST14, ZPP+16, ZYW+16, ZZWX11, AARP17, All11, ABB+12, ABB+13, BCJC+14, BH13, CCCLRO14, CCJ+11, DPOS16, DZA11, DHE+12, FMG12, GS14, GAI13, GD10, GHV17, HCB11, HS16b, HDH12, HZ13, HVS16, IHy15, KCI3b, KG11, KJM+17, KV15b, LC10, uLhY11, MS13, MS16, ME10, OSHG17, PG12, PLZ17, PNW+16,
consensus [DMJ17, SRA17, PLV+11]. consequences [KG15].
conservation [MB16]. Conserving [PH17]. considerable [LLD17].
Consideration [Fom11]. Considering [CSEMB+16]. Consistent
[DMJ17, POB13, BKŠ+11, BY11, BK17b, DK11, GBVA11, Hili13, HKR+14,
JSXH16, KT10, LBH+11, LCW12, ON14, SPS+12, SMP17b, SCSW13,
TYN15, VGG+11, YN15, ZBG11, BLKP12]. consistently [IM17].
consolidate [BK17c]. constant [AB16a, CS14, KSK11, KNP+12, MK17,
PS13, RAGLL11, ST1M7, Vor12, WOH16, WOH18, dACP12].
constant-distance [DBK17]. constants [MG11, OZLSBH12, Ray13, RSG14,
RKG11, Rui11, RRK16, SACdG14, TTR+12, Tsi14, WL14, XWW+11,
YS13, ZLL+10b, ZLL12]. Consistent [MB16]. Conserving
[PH17]. considerable [LLD17]. Consideration [Fom11]. Considering
[CSEMB+16]. Consistent [DMJ17, POB13, BKŠ+11, BY11, BK17b, DK11,
GBVA11, Hili13, HKR+14, JSXH16, KT10, LBH+11, LCW12, ON14,
SPS+12, SMP17b, SCSW13, TYN15, VGG+11, YN15, ZBG11, BLKP12].
considerable [LLD17]. Consideration [Fom11]. Considering
[CSEMB+16]. Consistent [DMJ17, POB13, BKŠ+11, BY11, BK17b,
DK11, GBVA11, Hili13, HKR+14, JSXH16, KT10, LBH+11, LCW12,
ON14, SPS+12, SMP17b, SCSW13, TYN15, VGG+11, YN15, ZBG11,
BLKP12]. consistently [IM17].
constituted [HDL+17, ZLY+16]. Constructing [Che17, HS16b, LG11, SWA13].
content [CGBK13, GWPJ11]. Contents [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].
context [CBG16]. continuation [PJ13].
contributions [JJH+13, ARRC15, BCNH+11, CGR16, CPN+17, ENKK+17,
WS10]. control [BVY+12, DPAB16, Hel13, HH16b, LPLB16, SR10, XYW+14,
ZQ14]. controlled [VGTL16]. Controlling [FWB14]. convective
[SBN13a, SBN13b]. Conventional [SHL+13, BKŠ+11]. conventions
[BCJC+14]. converged [FLM11, GR10a, KHWB17]. Convergence
[GS16, LT13, ZH12, AS10, BKŠ+11, GS15, ON14, RFHG10, SL17].
converges [SH11a]. Converging [OSR16]. conversion
[LDB+17, LGL+15a, LCB10, RVP+11]. convex [CLFRO18]. convolution
[SZTSM10]. convolutional [LHO17]. cooperative [DBG11].
cooperativity [RS14, AFJ16, JSW10, SM16a]. coordinate
[AMGB10, HSN14, Hel13, LL15, LL13a, MS10, WBN+13]. coordinates
[BK15, LKW+14, NCV10, PH10a, Sch13, VGV+11, YN15, ZBG11, BLKP12].
coordination [ASMS10, CRC13, HS16b, KJ10, Mor15]. copper
[JRSHP14, KKPT11, SBC+11, SPR+13, WC14, ASMS10, CPK12, HRJ+14,
HGHP14, HRJ+15, XWSW13]. coprocessors [WS13]. Copyright
[dCLFGL13]. crossing [LLSW14, QCR12]. crossover
[CSS17, KV14, MK17, SHMO11, VFRAR16]. crowded [MH17]. crown
[AvKSP16, HLB15, MWJ+11]. crown/ammonium [AvKSP16]. CrWO
[WMW11]. cryo [MKM+17]. cryo-EM [MKM+17]. Crystal
[Kri10, VM11, ASL+11, BCSCI+13, BCJC+14, Elk16, GMG+10, HB14,
HJ10, MCAG+16, NHF+10, NTNY15, OB+12]. crystalline [DOM+11,
DLSD13, DB12, EP12, EFOD13, GS12, DCOD13, RB13b, WDLG12].
crystallography [YW13]. crystals [HZSS17, KGH15, KLN12, KB16,
LPAS11, PLP+16, SFDE16, VECT12, You10]. CS
CTOCD [PC14]. Cu [NGAS17, Rab12, RHT+15, TS15b, WRG+17, AMK11,
CR14, CMID13, GEP+14, HSH15, Mor15, PGs+15, PXXW10, PH12,
RHT+15, SB10, WGN+16, WGLG+16, XP13, ZRCC11, ZSWL12]. Cu-O
[ZRCC11]. Cu-ZSM-5 [Mor15]. Cu2II [WGLG+16]. Cuby [Rez16]. CuCN
[TS15b]. CUDA [SR11]. CUDA-enabled [SR11]. CuE [TG12b],
curcumin [AMK11]. Curie [WMW11]. curing [LPMT17, PPH+14].
Current [ATM18, NS17, ABM+15, FNSF+11, GWT+17, HLBLC15,
PCLL11, PL18, PZM15, Vik11]. current-density [Vik11]. currents
[CP+17, RVB+12]. Curvature [LPLS16, RR12, NW17].
Curvature-dependent [LPLS16]. curves [BB11, LSH+11].
Customizable [AFBR17]. cut [DH14]. CuX [YS13]. CVD [NIIT15]. CX
[LGW12, EPH+15, ZYLL12]. CXH [CKL+11]. CXHM [LDJ+10].
cyanie [LZHH11, LLW12, TLY+12, VVBL17]. cyanide-chemosensing [LZHH11].
cyanides [PGs+15]. cyan [PKK17, TS10b]. cyanobacteria
[RCM+13a, RML+15]. Cyanovirin [VM11]. cycle
[HDl+17, SJD14, SOY12, dSDaR10]. cycles [UKS11]. cyclic
[CHZ12, LC10, PB14, RB12]. Cyclization [HPT16a, APA+14, LZL+16].
cyclizations [AARP17, DCHL12]. cycloadditions [YZN13].
Cyclobutadiene [SMF14, MCC11]. cyclized [QZ10a]. cyclodextrin
[DBG11]. cycloguanil [APA+14]. cyclohexane
[CRBO16, SNK16, SAv15]. cyclohexanes [SNK16]. cycloocta
[ABDGN12]. cycloocta-1 [ABDGN12]. Cyclooctaturae [DP11, SP13].
cyclopentadienes [LZHH6]. cyclopropenyliene [VVP12]. cyclosporin
CYP19A1 [VCM15]. CYP2A6 [ALW+10]. cysteine [CPK12, SDL14].
Cytochrome
[EH13, BS16a, MRR11, SLY+10, SOY12, TN10, TDP+12, VCM15].
cytochrome-P450-mediated [MRR11]. cytochromes [APA+14]. cytoseine
[JS17a, LZL+11, ZZY16]. D
[LDW13, OZLSBH12, RSKG14, UT14, YZ15b, AKMT11, BWKW10a,
BKW10b, DVP14, ETLS17, GMAT16, GSS13, GP12, LTT16, MA16,
MYT+14, MI11, MOP17, MH10, PSS14, PZBA13, RSKG14, TFQ+10,
YJN+11, YDL+10, ZLY+16, TS15b, YOB16]. D- [YJN11]. d-AO
[YOPB16]. **D-FFT** [MYT+14]. **D-galactosidase** [AKMT11]. **D-QSAR** [GMMH+16]. **D-RISM** [MYT+14]. **D-structures** [DVVP14]. **D/TIP3P** [SA10]. **D2** [LAHS16]. **d9k** [PNG10]. **damaged** [LZH+11]. **damping** [GEZ11]. **DAMQT** [KYG+15]. **dance** [JW16]. **dancing** [LL10b]. **Dancoff** [HH17]. **data**

[BRGN12, BCP+10, FN12, Fom11, HPT+16b, HM13, JZL+17, JS17b, LAS+14, MM+17, MCC12, RO14a, REL+14, RCM+13b, SB10, XW15].

**database** [PLAC11, XTG+11, XMSZ16], **databases** [CSSB11, OHPR17, ZWL13]. **DataPipeline** [FN12]. **dataset** [HZ13, KSM17]. **datasets** [GCC14]. **DBD** [YJZX13]. **DBeH** [UT14]. **DBU** [YZ+15, YZ17]. **DBU-H** [YZ15b]. **DCMB** [WX12]. **DDPredictor** [HL+13]. **deacetylases** [KC13a]. **dead** [SL10]. **dead-end** [SL10]. **dealing** [MFR10]. **deaminase** [WZQW10, ZZ+16]. **deamination** [ZZ+16].

**Debye** [GBFD12]. **DEC** [BK17c]. **DEC-RI-MP2** [BK17c]. **decamer** [DDP16]. **decarboxylase** [BEL+11]. **decay** [DPAB16, LCH10, LLI12].

**Decoding** [MBT14]. **decoherence** [CSEBM+16]. **Decomposition** [DBGO+17, AMAA+11, BMBJ11, FFA14, GS14, GCW16, ISN13, KNE11a, KRSC12, NJX+10, PS17, RSLML12, SSGS15, STM17, SKGB13, WWU12, WES13, dSDS12a, dSDS12b, dLC17]. **decomposition-based** [KNE11a].

**decouples** [FM10]. **decoy** [HYMZ16, LS11a, PHDH13, UCFR16]. **decoys** [BS+12, MP11]. **decrease** [DLZ15, SLY+10]. **dedicated** [CRS18, ZRCC11]. **Deep** [GHH17, GFPSD17, LOH17, LHD+14]. **deeper** [VIT+15]. **defect** [ZWP11]. **defective** [YZN13]. **defects** [HYL+11].

**deficient** [YLL11]. **defined** [JJAB16, GY10]. **definitions** [JYC+16].

**Definitive** [TCGNT18]. **Deformation** [WYL+15, Gav12, MRB14, WCY+11, WCT+11, dLC17]. **deformations** [HRM+13]. **Deformed** [CSAdOM17, TFQ+10]. **degree** [Clo15].

**dehydrogenase** [ZX11]. **deleterious** [XL+11]. **delineate** [SBT17].

**delocalization** [BK11, FV10, HS+11, Jan16, Mat14, SS13b, SSA+17]. **delocalized** [Alg17, HSH15, dLC17]. **DelPhi**

[DLSA14, LCA17, LLZ12, LPLA13]. **DelPhiForce** [LCA17]. **delatahedra** [LK16b]. **deMon** [LZdL+10]. **deMon2k** [BTT10]. **Denaturation** [IPAA11, FMG12]. **Dendrimer** [MJB12]. **dendrimers** [CAD16, HDH15a, HDH15b, HDH15c]. **Deng** [ASO12u]. **dense** [ASK18].

**Densities** [ATM18, HGCCGR+16, LP11c, MA16, REL17, dLC17]. **Density** [AMK11, CD13, CWH11, FPV13, FD16, GNGCA10, GPWJ11, INT18, JYS+12, KKKT11, LBGS16, LGW12, LBTV12, LPMT17, MWJ+11, Oht16, PPH+14, RB12, RSLML12, TS10b, WDLG12, WGN+16, YJ11, ZLZ14, ZYG+14, ZYW+10b, ZYW+10a, dSY12a, ALK+15, Ano15-19, AG12, ASS10, BY11, BLBG+13, Ben17, Boz18, BB1+11, BZB+13, BG13, CHG+16, CRZ+18, CDB10, CR14, CAA10, CEBO15, CQR16, CKH17, CSXZ17, CC11, CAP17, CNK97, CPL111, CBI11d, DH17, DWWC17, DII15, ED15, EPI12, FED17, FCP1M14, GA14, GHL17, GZL+12, GWJR18, GMG+10, GSS13, Gra15, GEG11, GAJ+17, Han11, HNWF07, HNWF12, HPT17, HEMCZE+14,
HLBLCCG15, HRMAL+13, HH16a, HH17, Hıı13, Höf14, HG10, HOK17, IKN13, IM17, JCP14, JLH+14, JW16, KD10, KB10, KSSH13, KOP+14, KGHK12, KB13, KZZ+16, KLN12, KYG+15]. density
[LL15, LCW12, LBT11, LHKS12, LWWG12, LH14b, LLH17, LZS+17, LK16a, MAK+14, Mat14, ME10, MKM+17, MFR+17, MJ10, NF17, NN18, NO16, NNK+16, NFI+16, NS17, ORZ11, OM12, OVPK15, PAK17, Pie14, Pil17, PW12, PZM15, QZ10b, RJPB12, RS13, RB13b, RG14, Rod13, RHPWS13, RHT+15, REV+17, Rui11, RSKG14, SPS+12, SPGJS+17, SH15, SS16a, SDF+17, SF+17, Sea10, SCW11, SDM+16, SEF+16, SE14, SH14, ST13, SHL+13, SPR+13, SZX13a, SZX13b, SMM15a, SMM15b, SMM+18, SKTT11, SZZS16, STS15, SK11, TldG+12, TN10, VGV+11, VAR12, VECT12, VV14, Viki11, VLI7a, VI17, VED10, Vybi6, WKC10a, WGL+11, WCWW11, WWU12, WWCL15, WHX+10, WL14, WTH+16, XYW+14, YLZ+10, YS13, Yu12b, ZTH+15, ZXS+10, ZSWL12, ZKE+17, ZDX11, ZLHH14, ZGS+10, dSdS12b, dSdLBNB17, dLC17, CDM10].
density-based [LZS+17]. density-density [LL15, LCW12, LBT11, LHKS12, LWWG12, LH14b, LLH17, LZS+17]. density-fitting [Boz18, Hil13].
Density-functional [Oht16, CHG+16, HNWF07, HNWF12, IM17, JCP14, KZZ+16, MFR+17, NF17, NN18, NO16, NNK+16, RHPWS13, SPS+12, VED10]. density-peaks [LZS+17].
deoxy [VM11]. deoxyribonucleoside [XVN17].
deoxyribonucleosides [RJWW12]. dependant [PNG10].
dependence [BRLS08, BRLS12, FE14, GZZ+16, KGO12, Lar12, LPE+10, LLTC12, MP17b, PZA15, PBE16, PS10, SGPJS+17, SY16b, AD10, MGWR12].
dependences [SMM+18].
dependency [DKT13, PHDH13].
dependent [AALCM11, BS16a, CHG+16, CP15, CKP10, DP15, EPD+10, GKK10, HNWF07, HNWF12, HG10, HYUS11, JYS+12, KCPMG12, LPLS16, LZ12, LZGS11, Mat10, NS10, PAK17, PPJ14, PVJ10, RHPWS13, REL17, SY16a, SFBFT17, Vik11, WHL+10, WHX+10, YLZ+10, ZXS+10, ZDX11].
deposition [SE14]. derivation [SCMA+17, VVV+15b]. derivative [MY17b, TPL+10].
Derivatives
[KTSW11, CWHH11, CZH12, CBTZ16, CROB16, HSZ+11, JS17a, JYS+12, KG11, KPL15, LWGZ15, LWWG12, MFR+11, M15, NS10, PC14, RVB+12, RFN15, REH13, SBR13, SZX13a, SZX13b, VVVJ15, VYV18, VSD10, WGL+11, WRG+17, WDP+12, ZsA10, ZWZ11, ZZ12, ZZZ11].
derive [RVP+11]. derived [CIKT13, GMMH+16, KSR+16, LZGS11, MCLD10, OSS10, PLZ17, REL17, SOYC12, SE14, TBSM12]. Deriving [CCYL11].
descent [MS16]. describe [HRCH16, RS13]. described [BM12, CCB15, KDS17]. Describing
[MKGA10, JCP14, JBSQ11, MY17b, VBD11].
Description
[FD16, MR17, BD12, BE16, Cam15, CRZ+18, LZLC13, MFR+11, PM13, PLH16, PVAM16, SRF+17, SSA+17, TKNN10, WWRSM14, WL14].
dercriptor [DFF+15, MA16, PRY17, TMJ15, WMW+10, Yap11].
descriptor-based [DFF+15]. descriptors
[FCL+10, FZL+15, GJMPAM+14, MH10, NKLJ16, PKIC11, RB13b, TTB+10,
Wei12b, YLCX10, Yap11, YDX16, ZWX16]. **Design**

[LCM16, Tak14, TZ12, VBD11, AM10, AFBR17, BAMR13, BEPM14, BPC13, CBP14, DPB+12, DPOS16, DGL+13, GS14, GMZ12, HHBY10, ISP+10, KSD+12, LABSG17, LBS10, MS16, PC11, SYDS11, SGM+13, Sti15, TKXT13, TRA+16, VVY17, VMP17, XHLH16, ZSB+11, ZWP11, ZYW+16, ZWS+10].

**designed** [BLL13].

**Designing** [BLL13].

**details** [MBA14, RSG+10].

Detected [TCPPC14].

**determined** [CHP11, IM17, YK13].

**Determining** [DSD+11, SGPJS+17, SDB+16, WOH16].

Developers [GKV+13].

**Development** [GLB16, GMMH+16, LLJ12, MMB+17, MMZW14, MCP18, RZG+13, RLD12, SC17, TNYN16, WOH16].

Developments [YWJ+16].

**Deviation** [CSAdOM17].

**deviations** [HDL+14, KG15].

**devices** [DJX+11b, DIX+11a].

**Dewar** [Bac12].

**DFT** [CLFRO18, SIG+15, YJ17, ZZY+16, AALCM11, AR10, AF14, ASMS10, BTMS12, BIL10, BTB+11, CLFRO18, CMM18, CCB15, CH10, cCVG+14, CXS10, DJD12, EFAC13, FVP14, FRPS14, GMASBF16, HSH15, HRJ+14, HRJ+15, HBI+17, JRSHP14, KG15, Kar17, KT12, KKL+13, KM13, KP10, LEDLOld17, LRBB12, LZX+10, LZHH11, LZX+10, LSH+11, LYSS11, LZLC13, LH14a, LLSW14, LCM+14, MMS16, MTD16, MG15, Mat10, MS11, MVKS10, Mor15, MCK17a, MCK17b, NKJ16, NC12, NMLD13, PTK11, PHK14, QLYL10, Re17a, RDF+11, RS14, RRC+15, RN17, REL17, RKB+14, RK13, SRF+17, SWM10, SRL+15, SDL14, TSNC+17, TG12b, Tsi14, TS15b, Tsi17, VVJ15, VECT12, VAMS14, WKL12, WYBW12, YZGS14a, YSRSS10, YZ15b, YXZ17, ZCK+16, WZGO16, ZZWT12, dSDdAR10].

**DFT-based** [NKJ16, NC12].

**DFT-derived** [REL17].

**DFT-MD** [GMASBF16].

**DFT-predicted** [WKL12].

**DFT/MM** [RN17].

**DFT/TV** [LXZ+10].

**DFT/TDDFT** [LXZ+10].

**DFTB** [SA10, FHT+15, MR17].

**DFTB/MM** [RN17].

**DFTB3** [KW15].

**DGeCl** [MCLD10].

**DH** [SGPJS+17].

**DH2** [SBW12].

**di-mannose** [NM11].

**di-tetrazine-tetroxide** [MCAG+16].

**Diabetic** [DHOG13].

**diabetes** [PC11].

**Diagnosis** [MC12, TDKT10].

**diagonal** [BMBJ11, KTK17].

**diagonalization** [BKŠ+11, HKR+14].

**diagonalization-free** [BKŠ+11, HKR+14].

**diagram** [OV14, VED10, ZY14].

**diagrammatic** [WWD14, YD17].

**diameter** [AS15a, KGHK12].

**diamond** [JWO15, WGN+16, WGLG+16, ZSL+11].

**diamond-like** [ZSL+11].

**dianion** [DP11, GRD+10, YZGS14a].

**diarylalkyl-imidazole** [NS10].
[NS10]. diarylalkyl-triazole [NS10]. Diarylbibenzofuranone [SFA17]. diaryldichalcogenides [ZWGO16]. diastereoselectivity [AARP17].
Diatomic [ATM18, LS11b, Tsil4]. diatomics [TG12b]. diatomic [CPN^+17].
dielectric [DOM^+11, DSF17, JLCA17, KCPMG12, PS13, WXL17, YHW17]. Diels
[BJSI12, CC18a, FB14a, GMDA^+12, LZH16, ORZ11, ST13, dSVdM^+16].
difference [LLH17, WL10, Yon16, ZRCC11]. difference-dedicated [ZRCC11].
differences [BVC13, GO13, HDL^+17, KHWB17, LGL11, PM18].
Different [PH15, BRGN12, Di15, FZL^+15, GO13, GR11, GFPS17, GMPP12, Kar17, MCS11, MC12, MPA12, NMLD13, NOKJ16, RHNN10, Rao11, SLP^+12, SIG^+15, TSNC^+17, UT15, VVY18, ZR10]. Differential
[HHT^+13a, HHT^+13b, CJL^+13, MY17a, MY17b]. Difficult
[RJS17, VDVR14]. diffuse [YCGA10]. diffusion
[CPV^+12, CC12a, GC11, RSL13, ZW17, WH11]. diffusional [MBR^+15].
Diffusive [SM16b]. digitized [YNH^+17]. dihedral
[CYG^+15, OZ14, SZBM13, WES13, ZRL^+15]. dihedrals [LDH^+14]. dihydro
[RS17a]. dihydrofolate [RKDM14]. dihydrogen [PM13, UT14, WHX^+10].
dihydrogen-bonded [UT14, WHX^+10]. dihydrogen/hydride [PM13].
dihydropyridine [YZ15b]. diimide [MCC11]. diiodide [AARP17].
diiodide-induced [AARP17]. diketopyrrolopyrrole [HLWD15].
diketopyrrolopyrrole-based [HLW15]. dilanthanide [ZLZ14]. dilute
[KVR10]. dimension [HKRS11]. dimensional [BPLL12, KYT^+17, KRC12, KTO13, MB16, PJ13, SG10a, TYN15, TCX^+13, TKC^+11, ZWX16].
dimensionless [MS10]. dimensions [CHC^+13, HAL14, SRL^+15]. Dimer
[LWL^+16, ARRC15, ANH^+11, BPPS17, CBTZ16, FCL^+10, FMNC11, KCB^+12, LCB10, PD11, SKY^+11, Tac17, WWKS16, YCGA10].
dimeric [PS14]. dimerization [DS^+11, KAR12, TLA10, WJX^+10]. dimerization/
oligomerization [KAR12]. dimers
[BCNH^+11, BWKW10, BWKW10b, CLFRO18, CK10, JKS^+16, LJW11a, LMI^+14, PVS12, RS13, SZS16, VT14, Zha11]. Dimetallic [ZYG^+14].
dimethyl [GC11, WLC12, ZSW12]. dimethylaminoazobenzene [KP10].
dimethylaminophenyl [YLZ^+10]. dimethylnitrosamine [FPA14].
dimyristoylphosphatidylcholine [ML14]. dinitrophenol [MIS^+15].
dinuclear [OS10, QLYL10]. dioxygen [GM17]. dioxygenoisilane [KL16].
diphenyl [KCPMG12]. diphenylamine [PZ10b]. Dipole
[SC17, Kop17b, QZ10b]. dioxygen
[DHF^+11, RSL16]. diphenyl [GKR13, Ray13, RKG11]. diphenyldiiline
[KLN16]. diplatinum [KT12]. Dipolar
[YSB12]. Direct
[LZY12b, WAM17, FF11, FSSW17, JCG^+10, RSB^+13, Yu12a, LLHM16].
WdVN12, WZ17, XML+15, ZL11, ZWL13, ZSB+16, dVZ17. docking*
[MBFG15, MIS+15, SV15]. DOI [Ano15-59]. Domain
[KNE+1a, AC11a, IMK+16, MBT14, RZ16, SFBT17]. domains
[FCPJ14, OOK11]. dominant [Hua16]. done [LRvE17]. donor
[DGL+13, Gil11, Lu11, MSV16, MIS+15]. donor- [MIS+15]. donors
[LC10, TZ12]. dopant [SRL+15]. doped
[GAMAC+14, LLC17, PGC12, TN12, VS14, WMW11]. doping
[HYL+11, LLD17, WMW11]. DOT2 [RTP+13]. dots [DPAB16, WAB17].
double [Alg17, BE14, CCB15, CGR16, CC11, FC16, KM13, LBH+11,
LYC+13, LLL+12, SGPSJ+17, SP13, Sea10, YYT12, ZLY+16].
double-Hybrid [CGR16, LBH+11, SGPJS+17, Sea10]. double-wall [BE14].
doubly [CSXZ17, SZX13a, SZX13b, ZWLX11]. Douglas [YS13]. DOX
[RCR+16]. DPO [WGL+11]. DPPC [LBDP12, vRWGS17]. DPT
[BH13, BZH14]. Dramatic [MLY+13]. Draw [LBB+15]. drawback
[BRGN12]. Drew [IPAA11]. driven
[BSL11, BG17, DSM+11, HXM+16, KC13b, LZL+13, LLL+12, REL17].
driving [RN17, YZ17]. Drude [LRvdSM15, Ric16, SM14b, ZM10]. Drug
[GHSM10, MBA14, FLM11, GMASBF16, Ibr11, ISP+10, PC11, PVJ10,
VHA+10]. drug-like [VHA+10]. druggability [LG14]. drugs [PPUBGD10].
DSCs [YJN+11]. DSPMP [FZL+15]. DsRed.M1 [SGDT10]. DSS
[GZM11]. DTTO [MCAG+16]. dual [JCG+10, MA16, TMJ15]. Duncanson
[Bac12]. duplex [HDK+12]. Durandal [BSZ+12]. during
[GNDA+12, LBC+12, MJLV14a, MJLV14b, PNG10, RSKG14, dCDP15].
dyad [KP10]. dyads [KKC+15]. dye
[ACS12, JYS+12, LZZ+15a, SLP+12, YJN+11]. dye-aggregates [SLP+12].
dye-sensitized [ACS12, JYS+12, LZZ+15a, YJN+11]. dye-sensitizer
[YJN+11]. dyes [DBM+17, VAA14, WJG+13, YJN+11]. Dynamic
[LKL10, SFA17, TNYN16, AKK+16, BS10a, BMB31, CVT+11, ESM+12,
GMB+11, Hel13, MB14, NYN17, OPR16, Vor12, PBDW11]. dynamical
[ALH+10, EFOD13, Ham11, VPR10]. dynamically [HS17a]. Dynamics
[CPV+12, LK13, MFEM16, AAS18, AALCM11, AG11, AS15a, Aki16,
ASL+11, ABD11, APK14, AB16a, ALH+10, BHB12, BSL11, BDP11,
BJ12, BW15, BF17, DMN15, BMBJ11, Bow16, BEL+11, CTR13, CS14,
CH16, COOH14, CCW+10, CHKR10, DASA15, DGH+11, DSD+11, DZT11,
DLZ15, EP10, ETL17, EFOD13, FOM13, FBEM11, GBL+11, GDV17,
GR11, GZ15, GCW14, GGM+12, GP11b, GC11, HZ11, HS17b, HCD+10,
HP10b, HPT17, HPSK12, HJ10, HWWL17, HRID16, HC14, IUK+11, ISK14,
IM17, JJ10, IPAA11, JIS13, JA10, JBSQG11, JCG+10, JAH+17, JWST10,
JMS14, JS17b, KCK+17, KVC+11, KUDG12, KGHC15, KDB13, KB14a,
KNE11a, KERY+16, KLOS10, KJM+17, KSR+16, KG13, KV15a,
KVR10, LL15, Lar12, LWK+14, LH11, LJ+12, LL13a, LRvdSM15, LCH10,
LYC+13, LMI+14, LPE+10, LLTE12, LZS+17]. dynamics
[LPLB16, LTT12, LBDP12, MBT14, MKS+12, MSC+10, MJC14, MN15,
MCRL17, MFEM15, MADWB11, MKM+17, MB16, MHRR11, MO17, MIOM13, NPTS16, NST14, NFPD13, NFG+13, NNK+16, NHK+13, NTNY15, Oht16, ON14, OGL10, OCL11, OLY17, OT12, OCW+15, PMC+17, PSS14, PAK15, PH15, PL14, PM13, PD12, PHT17, PVZ13, PS10, PVAM16, RS12, Ras17, RO14a, RO14b, RFN15, RR14, RdA12, RVdB16, RLG14, REL+14, RŠRR15, RSB+13, SHMO11, SLT+15, SMW10, SSWX14, SOM+13, SIJ, SR18, SYN+12, SM16b, SK13, SKMS13, SFLG+17, SLLL13, SJ16, SV11, SBvG14, SAvg15, Tac17, TNY16, US11, Vor10, VM11, WKL12, WBN+13, WAM17, WC11, WHL+10, WH11, WWKS11, WLC12, WES13, WG14, Wu10, WBVE16, YPyD13, YJXZ13, Yon16, Yu12a, ZZY16, ZX11, ZDKM12, ZBP11, ZP13, dCLFGL13, dSVdM+16].

Dynamics-based [Vor10]. DynamO [BSL11].


Editorials [BEFS13]. Effect [ABD11, CBG17, CS17, GEG11, HYL+11, JZ12, OBW12, RRF11, VS14, dALdS+15, AB10, CSHK16, CD11, CXS10, DKT13, DJX+11b, DLW12, FCOGM12, FHK+12, GFGS18, HLBBCCG15, JWO15, JYS+12, KTT16, KCL+14, KLN16, LlyG10, MTV12, ONTT16, RWR+13, SLT14, SBC+11, SY16a, UT15, VLGK+17, WDLG12, ZJM13, ZLL+10, BLG10, CC11, IYK11].

Effective [GKV+13, IM17, YZ16, AASP18, DMN15, CVG14, DMN14, GA12, KS13a, KS15, LCM+14, PHC13, PRY17, PS13, RLD12, ŠSB+16, UCFR16, WX5+12, YZZ16, YZ15b, ZKH+10]. Effects [CS14, JAH+17, LGOM+15, LCH+15, Mor15, SEM12, Tac17, YCK16, AS15a, AK10, AS18, BBF+11, EPH+13, FAA15, FD16, GMG+10, HS16b, HLBBCCG15, INT18, JMXP+16, KG11, KYCL11, LGVA14, LHT15, LWD13, MKGA10, MBC11, MRK11, MLY+13, MCUJ15, MGS+16, NASH15, ORZ11, OSHG17, OCW+15, PDMT10, PCI14, RMGB11, RRK16, SSWX14, SMP17a, SFLG+17, TM16, TY115, TY10, UT14, VKAM12, WXY14, YNH+17, YJ11, ZPP+16, Zha11, ALW+10, THP+15].

Efficacy [LC17a]. efficiencies [RO14a]. Efficiency [AC11b, BB11b, BB11c, FE14, GBSE11, XFG+16, AC12, GSHM10, LY10, LWL+11, LZL+15a, MKGA10, RO14a, XFG+15, vLBBR12]. Efficient [AB16a, BC13, BAS14, Cas13, DMAH15, DBF14, EP10, GCWS15, GPK12, Ham11, HNS16, HDL+14, HHWL17, JMS13, LZ11, LGKS17, MKS+12, NYN17, PSS14, PAK15, Ran12, RJS17, SS16b, TJB12, WHAS+16, WMI2, ZZ14, ZKE+17, AM10, BW11a, Bose18, CBP14, CHG+16, CY09.
CY13, CMS13, DS15, DGL$^+_{13}$, GREA11, GWZX12, HDL$^{+}_{17}$, ISK14, JZ17, KB11a, KV15b, LFB14, LPK16, LLZA12, LZZ$^{+}_{15a}$, LZZ$^{+}_{17}$, LAS$^{+}_{14}$, NPTS16, NN18, OK16, PW12, PBG17, Ran13, RR14, Rod13, RSL16, SCOJ13, SA13, SSMW09, SCSW13, SWB$^{+}_{12}$, Sun15, TO10, WJG$^{+}_{13}$, WOH18, ZWP11, Zha12b, Zha12a, vLBBR12, WHAS$^{+}_{10}$]. Efficiently [WES13, ASMS10, DDK14]. egg [Pla11, ZP13]. egg-box [Pla11]. EGRAD [vW11]. Ehrenfest [Dil15, FED17]. eigensolver [KZZ$^{+}_{16}$]. eigensolvers [ZVY$^{+}_{15}$]. eigenvalue [HLXH17, HLXH18]. eigensolvers [ZVY$^{+}_{15}$].

Electric [GH16b, LL13b, B LFZ13, B LBG$^{+}_{13}$, BS10a, CXS10, GH16a, KZK$^{+}_{12}$, MRB14, SH15, SLX$^{+}_{15}$, Yan11, YJ11, YCK16, ZSLL17].

electrochemistry [DSK17].

electrochemical [SIG$^{+}_{11}$, SGH$^{+}_{16}$, YJ11].

electrochemical [SIG$^{+}_{11}$, SGH$^{+}_{16}$, YJ11].

electrolytic [SV11].

electrochemical [SIG$^{+}_{11}$, SGH$^{+}_{16}$, YJ11].

electrochemical [SIG$^{+}_{11}$, SGH$^{+}_{16}$, YJ11].
electrophilicity [YB16]. **Electrostatic**

[CLA16, LP11b, MLZZ12, Sch18, WFZ+18, BCNH+11, BSF18, BK13, CCC+11, CS14, CPK12, CB1c, DLSA14, GBL+11, HOK17, IO13a, KTN10, KYG+15, Lar11, LCA17, LCM16, Mat14, PVJ10, RB13b, TY10, VMRSH+17, VVY18, YKO+11, YWJ+16, YMP14, YZL+15, ZDZM13, ZBP11, KGM12]. **Electrostatics** [BSG18, CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NLP+16, SDZ17, SWPR11, UHH+11, XYX17, YMP14]. **element** [BCCO10, GPK+16, RMGB11, TG12b, TCX+13, XYX17]. **elementary** [LPLB16, Zim13]. **Elements** [TKN13, BV14, CWZB10, Hil13, JJJ16, LFB14, SK15a, TDKT10, Tsi14, WS12, XhD15]. **elevation** [HH10]. **ELF** [RSKG14]. **ELI** [BWKW10a, BWKW10b]. **ELIA** [BWKW10a, BWKW10b]. **elimination** [SL10, dCDP15]. **Elisabeth** [Ihl12]. **ellipsoidal** [DGB+13, LDG+15]. **Elongation** [OLA15, MKGA10]. **Elongation-MP2** [MKGA10]. **Elucidating** [HNHR13, TDP+12]. **Elucidation** [CPLL11, TNYN16]. **embedded** [DSF17, GMG+10, HSH15]. **embedding** [CCB15, ESM+12, HH16a, HH17, HfF14, HOK17, KSR17, NOKJ16, RR12, SDF+17, SS16b]. **emerges** [MNNK10a]. **emission** [LX11, MCLD10, PLP+16, SGWA17, WDP+12, ZLL+10]. **emitted** [PE11]. **Emphasis** [RCM+13b, PD11]. **Empirical** [BA11, DLMH12, KLN12, Hil13, JJJ16, LFB14, SK15a, TDKT10, Tsi14, WS12, XhD15]. **employing** [GP11b, MLCD11, TG12b]. **empowered** [BPLL12, RLHL12]. **enabled** [Aou16, BK17c, KYG+15, LL10a, SR11]. **enables** [KK17a, XHLH16]. **Enabling** [PHH+12]. **enamine** [AS11]. **Enantioselective** [ORZ11]. **enantioselectivity** [OAN15b]. **encapsulated** [EOO+16, STS15]. **encapsulation** [YDGZ15]. **encoded** [SL10]. **encoder** [LDH+14]. **end** [HDL+17, SL10]. **ended** [RJR14, Zim15]. **endo** [FB14a]. **endochemical** [FL15, GLF16, MCK17a, MCK17b, ZSL+11, ZYG+14]. **endochemically** [DM15, VIT+15]. **endothelial** [JAH+17]. **endpoint** [BB11a]. **ene** [GRCL12, FB12]. **enediyne** [DCHL12]. **Energetic** [JW12, CG15, MCAG+16, PBG17, SLHW09, TPL+10, YSRSS10, ZZWX11, ZYL+12]. **Energetics** [SFM14, BK17a, BMFG16, DSF17, GAJ+17, HEM+17, JJH+13, KB13, MP13, MBRC16, OCW+15, SJ11, SNS16, SL17, SDB+16, ST13, SFBT17]. **energies** [AF14, AS14, AG12, BW11a, BFL14, BVHH17, BS16b, BE16, CHG+16, CDM13, CH10, CTP13, CBC16, DHO13, DM17, DHP+11, DPOS16, FGM11, Gi11, GP11a, Grl13, HAKG10, HH10, HH11, HLW+17, HHWL17, IK113, KSH13, Kar17, KSM17, KJDB12, KB11b, KYP13, LJ11a, LW11, LHHW14, LH14a, MCS11, MS13, MSK12, MBE16, MMJ10, NW17, NMF+14, OBW12, yOTu16, OAN15a, ORS16, PGCT+12, PP14, RLJD17, RDDS10, RAR+11, RO14b, RZ16, RR14, Rob13, RJS17, SRR16, SK12, SHL+13, SOD+11, STM+15, SGWA17, TS14, TS16, UD12, VVG13, VECT12, VM11, WBT10, WS10, WJG+13, WG12, WX12, YAS13, YMP14, ZZ14, dALD+15, dRBO13]. **Energy**
epoxides [BCP+10]. epoxy [LPMT17, PPH+14]. epoxy-carboxylic [LPMT17]. epox-phenol [LPMT17]. equation
[BCCO10, CD16, CLA16, Fer13b, Fer13a, FCE15, Fra15, Fra16, KK17b, RSLS13, SK15a, SM16a, SG10a, WBVE16, XYX17]. equations [BYE+16, ZR10]. equilibrated [WHAS+10, WHAS+16]. equilibrating [OPR16]. equilibration [LBDP12, SMP17a]. equilibria

F [CXW14, CXS10, GPK+16, GTK10, HBL12, LZJ+11, Li14a, Li14b, PMG+16, Rab12, STM+15, TFQ+10, TFQ+11, TCPC14, WJL+10,


FEW [HG13]. FF [LGW12]. FFLUX [FP17a, FP17b]. FFT [MYT+14, WS13]. field [AKMYB18, AJR16, ALH+10, BKŠ+11, BCSCJ+13, BCJC+14, BY11, BW15, BF17, BK7b, BBG+18, CRC13, CIKT13, CYG+15, CZAF17, CLC11, CB11b, CB11c, CK17, DPNM11, DGPM14, DFF+15, DMAH15, DP15, DGB+13, DL215, EPD+11, Gar12, GSD10, GZM11, HH11, HKR12, HLH+12, HRR+14, HM13, HJLV16, HCP15, ISO+13, IHJ+13, JSXH16, KLJ+17, KSK+11, KT10, KMSL10, KVR10, Lar11, LVD13, LC17b, LPS+13, LPE+10, LN15, LLG10, Lg13c, LL13d, LDG+15, MRO17, MBC11, MSS+13, MTvG12, MBE16, ML13, MHRR11, MP17b, NTTY15, ON14, PHC13, PLZ17, PG15, PZCL16, PH16, PV10, PS10, PNG10, Rod13, SH15, ST11, SM14b, SK17, SZBM13, Sic15, SS13c, SCSW13, SM15, SYZ+17, SBGv14, Tak14, TYN15, VHA+10, VPR10, Vik11, VLGL17, WX17, WTH+16, WC14, WZK+13, WDH13, XP13, XVA+16, Yan11, YWZ14, YJXZ13]. field [YJ11, YN15, YCK16, YHV12, ZSLL17, ZL11, ZSYH12, ZDKM12, ZP13, ZM10, ZCGM11]. field-based [HKR12]. field-dependant [PNG10]. field-dependent [DP15]. fields [ASK15b, BSY+12, BAS14, CCLP12, CPN+17, GCW15, GMMH+16, HDP14, HJ10, JYC+16, KWL+16, LZZ+11, LGS11, LGL1, LTP11, LD12, MSh+10, MSK+12, MS15, ST11, SEM12, VV+15b, VHA+10, WKC+10b, WLC12, WG12, YPKB12, ZRL+15]. fifth [KM13]. fifth-rung [KM13]. file [SY16b]. files [MSK+12]. filter [MH10]. find
LH14b, LLH17, LPMT17, MAK+14, MWJ+11, MFR+17, Mor15, MMJ10, NF17, NN18, NO16, NNK+16, Oht16, ORZ11, OM12, PAK17, PPH+14, Pie14, PD11, QZ10b, RJPB12, RS13, RB12, RSLML12, RHPWS13, RHT+15, Rui11, SPS+12, SH15, SFG+17, SCW11, SBT17, SEF+16, SE14, SH14, ST13, SHL+13, SPH11, SMM15a]. functional
[SM15b, SMM+18, SKTT11, SZS16, STS15, TLdG+12, TG12a, TS10b, HV14, Vi11, VL17a, VL17, VLGK+17, VED10, WKC10a, WHL+10, WCCW11, WDLG12, WYT17, WHX+10, WL14, WTH+16, WGN+16, XYW+14, YJ11, YLZ+10, YS13, ZXS+10, ZWLX11, ZSWL12, ZLZ14, ZDX11, ZYG+14, ZYW+10b, ZYW+10a, ZLHH14, ZGS+10, dSdS12a, dSdS12b].

LH14b, LLH17, LPMT17, MAK+14, MWJ+11, MFR+17, Mor15, MMJ10, NF17, NN18, NO16, NNK+16, Oht16, ORZ11, OM12, PAK17, PPH+14, Pie14, PD11, QZ10b, RJPB12, RS13, RB12, RSLML12, RHPWS13, RHT+15, Rui11, SPS+12, SH15, SFG+17, SCW11, SBT17, SEF+16, SE14, SH14, ST13, SHL+13, SPH11, SMM15a]. functional
[SM15b, SMM+18, SKTT11, SZS16, STS15, TLdG+12, TG12a, TS10b, HV14, Vi11, VL17a, VL17, VLGK+17, VED10, WKC10a, WHL+10, WCCW11, WDLG12, WYT17, WHX+10, WL14, WTH+16, WGN+16, XYW+14, YJ11, YLZ+10, YS13, ZXS+10, ZWLX11, ZSWL12, ZLZ14, ZDX11, ZYG+14, ZYW+10b, ZYW+10a, ZLHH14, ZGS+10, dSdS12a, dSdS12b].

general [BSL11, EWK+13, FNSF+11, HSN14, Ish12, NLP+16, PH17, RJP14, Sun15, VHA+10, YHVM12]. general-contraction [HSN14].

Generalized [GHI6b, KCPMG12, AB16b, BSPP+13, DSF17, FCE15, GH16a, LL10a, MA16, PS13, SZTSM10, SSBW14, VMP17, WWKS11, WHM10, WBVE16].
generate [MPA12]. generated [HWLW11].
generation [ADF+10, MPA10, RVL11, CAD16, GMSdG15, HGY15, KLJ+17, KSH+17, LTT16, RB13a, TDP+12, WHHJ13, ZCGM11].

generators [MPA12, RvL11, CAD16, GMSdG15, HGY15, KLJ+17, KSH+17, LTT16, RB13a, TDP+12, WHHJ13, ZCGM11].
generators [MYT18, Gar12, GPM17].
genes [YS10].

GENESIS [KJM+17]. genetic [AC12, CB11b, FRLN10, LLJ12, NC12, RSL16, SHMO11, WMW+10, YVEI+17, LMA15].
GenIce [MYT18].

GenLocDip [GH16b]. GeO [DLSD13].

Geometric [MK11, CDB10, CDBM11, EHI3, FXC+13, HHT+13, LLFH16, REH13, TCC+13].

Geometrically [RJ1+11]. geometries

geometry-dependent [EPD+10]. Germanium [GSMM15, ALH+10].

GGS [SA10]. GLYCAM06 [SA10]. GLYCAM06/TIP3P [SA10].

Glu [EJ13].

Glycosaminoglycan [CHKR10, SA10]. glycosidic [HH11].

glycosyltransferase [RN17]. gbh [Spr10]. GMCT [U12].

GneimoSim [LWK+14]. gold [Ano15-58, BH14, CCJC10, FHT+15, GAMAC+14, Li14a, Li14b, LHKS12, LH14b, MFR+11, MG14, MBFG15, SRR16, SKTT11, YLL11].

GP [SA10]. Glycan [JS+11].
glycine [DB12, DP15, FCD10, MC10].
glycoconjugate [LABSG17].
glycoproteins [JS+11, PFVL14].
glycosaminoglycan [CHKR10, SA10].
glycosidic [HH11].
glycosyltransferase [RN17].

GmbH [Spr10]. GMCT [U12].

GneimoSim [LWK+14]. gold [Ano15-58, BH14, CCJC10, FHT+15, GAMAC+14, Li14a, Li14b, LHKS12, LH14b, MFR+11, MG14, MBFG15, SRR16, SKTT11, YLL11].

GP [SA10]. Glycan [JS+11].
glycine [DB12, DP15, FCD10, MC10].
glycoconjugate [LABSG17].
glycoproteins [JS+11, PFVL14].
glycosaminoglycan [CHKR10, SA10].
glycosidic [HH11].
glycosyltransferase [RN17].

GmbH [Spr10]. GMCT [U12].

GneimoSim [LWK+14]. gold [Ano15-58, BH14, CCJC10, FHT+15, GAMAC+14, Li14a, Li14b, LHKS12, LH14b, MFR+11, MG14, MBFG15, SRR16, SKTT11, YLL11].

GP [SA10]. Glycan [JS+11].
glycine [DB12, DP15, FCD10, MC10].
LBGS16, LFN+10, RSG14, SFG+17, SSMW09, SLG15, vLBBR12. **grafting** [KKR+13]. **grain** [SOM+13]. **grained** [BLKP12, CAD16, HHWL17, JC16, KCK+17, KVQC+11, KLS10, KMLS10, LZ12, LZX16, LZZ14, LZLMP16, MSL10, MBC11, MBC13, NST14, RSG+10, SLX+15, SDZ17, SJ17, SM15, SAvG15, WBF17]. **graining** [BJP15, GMPB12, ML14]. **Grand** [HLvdV13, PHH+12]. **grand-canonical** [PHH+12]. **Graph** [WSH10, DH14, GPGSM11, GPGSM12, Ihl12, MCC12, PShPE+10, Pog10, RPnP10]. **graph-based** [DH14]. **Graph-theoretical** [WSH10, PSdPE+10, Pog10]. **graphane** [YZZ+17]. **graphene** [CMM18, dRCFGRB18, DJX+11b, DJX+11a, JWO15, LWZK13, LCM+14, PL18, RRK14, SDF12, WCT+11, WZW15, WYL+15, WTH+16, YSSB12, YZZ+17]. **graphic** [HASR+12]. **graphical** [All11, GBL+11, HZY+10, LLLC11, LBB+15, PVZ13, SEF+16, STH+10, WSGN11, WS13, YWJ+16, YDL+10, YN15, YS10, ZKE+17]. **graphics** [AB16a, AB16b, BDTPI11, CKKK16, EP10, HKR12, HEMCZE+14, MSSP17, SR11]. **graphite** [Fom13]. **graphitic** [LL13b]. **graphs** [AGR11b, RNP13, RNVP13, SOJ14]. **Grätzel** [VÅ14]. **gravitational** [DS15]. **Grcarma** [KG13]. **green** [LWL+11, NSO+14, PGW+17, yOTn16]. **Gregori** [Ihl12]. **Gregori-Puigjané** [Ihl12]. **Grid** [BAMR13, HEMCZE+14, KP11, LZ11, LLZA12, MMM+16, RLLHL12, dVZ17, CM13b]. **Grid-based** [BAMR13, HEMCZE+14, KP11, LZ11, LLZA12, MMM+16, grids] [DH17]. **Gro2mat** [DDK14]. **GROMACS** [AG11, Abr11, Gar12, GP11b, KPF+15, LRvdSM15, PHH+12, TKT11, KWG15, DDK14]. **GROMOS** [HH11, HHL+12, KAG+12, LGL11, LvG13c, MRO17, MSvG12, PLH16, PFVL14, SBV10]. **GromPy** [PHH+12]. **ground** [BBI+11, CCM15, FAA15, GCM15, HH16a, Kop15a, LLBO12, LYY+13, LX11, LS11b]. **ground-state** [HH16a, Kop15a, LLBO12]. **group** [Alg17, CAP17, Dry14, EHSPT16, FC16, GZQM16, GPK+16, Gil11, GWZ15, HB14, JJJJ16, LZ11, LZ11, MSL16, RLLHL12, dVZ17, CM13b]. **Grids** [DK12, Tsi14, VDVR14, WS12, XhD15, LdSRR16]. **groups** [Kan15, KV15b, LPS12, TN10, WGL+11]. **growing** [JZ17, Zim15]. **growth** [DWZ+17, FCL+10, LL10c, LZLMP16, MZZ11, OME16, RS14, WC11, XYW+14]. **GRRM17** [MHT+18]. **Grubbs** [RS17b]. **GSK3** [LJL+11]. **GTKDynamo** [BTA+13]. **GTP** [SS13c]. guanidine [HRJ+14, HGHP14, HRJ+15, JRSHP14]. guanidinium [CCCLCRO14]. guanine [BZH14, CBG17, LZH+11, PDMT10]. guanine-cytosine [LZH+11]. guanines [WGL12]. guanylthiourea [MAPB10]. guest [CC18b, OAN15b, YDGZ15]. GUI [WCJ+14, HBJ+17, JCL+17, KLJ+17]. guide [BS15, GKV+13]. **guided** [OCL11, WVE16, YVE1+17, Yon16, ZC14]. guiding [HS17a]. **gWEGA** [YLGX14].

**H** [B18, BS16b, CCS10, CG12, DM15, GPK+16, HZ11, HSY+11, HVS16, JLS+10, JLH+14, LLL+11, LDSSR16, LAHS16, LDW13, LLQ+12, MCAY15, NMLD13, OPR16, PMG+16, RMPAM15, SNKD16, STS+10, Tak11, TSJ+10,
TFQ+11, UT14, VIT+15, VV14, WKC10a, WKCL12, WHL+10, WWKS16, WCL+11, XFX+16, YKH15, YZ15b, YZZ+17, ZYLL12, AS15a, Ben17, BS10b, CK10, CKL+11, Chu10, DHE+12, GTK10, GS11, HZ11, HRL11, KTT16, LJW+11b, LWD13, Nix13, OKIS17, PTK14, Pie14, Pon10, STS+10, TS15a, UT15, WGL12, WvRSM14, XhD15, YZ15b, YZZ+17. H- [Pon10].

H-atom [BS10b]. H-bonding [WGL12]. H-C-C-H [YZZ+17, YZZ+17].


half-sandwich [TS15a]. half-saturated [WDZN16]. halide [Li14a, Li14b, NC13, ZW17+10b]. halides [FWB14, PGS+15, VVP12].

halobenzene [EPH+15]. halofullerenes [TFQ+10]. halogen-bonding [HDB15]. Halogen-Bonds [WFZ+18]. Halogenated [HvM17, EPH+13, HvM16].

Hamiltonian [IO13b, MGWR12, OZ14, VFRAR16, YS13]. Handling [IO13a, MBC13].

Hardness [SBR13]. Hardnesses [YB16]. HArF [LZJ+11, WZK+13].

Harmonic [LBH+11, Aom15-58, BH14, CHC+13, LLH17, WAM17, WTH+16].

Hartree [BY11, CKKK16, CB11d, FRN15, HJKJ13, IYK11, Mat10, PB14, PW12, RH12, SG13, VL17a]. harvesting [KDR+18]. HBaH [UT14].


Heck [dSdLB17]. heights [BS10b, GAJ+17, KG15, ZW17]. Heine [Spr10]. Heisenberg [CME11]. helical [FCD10, KB14a, LHKS12, LH14b, McvdV13, MV17, PRP15].

helices [DS17, HHT+13a, HHT+13b]. helix [CCOH14, LMI+14, WXL+12]. heme [FBEM11, INT18, LS11b, PBC13, SOYC12, SH17, TN10]. Henkelman [QB11].

Henry [QLYL10, VKTRJ15]. HEPT [ZsA10]. heptagon [GZH10].


heterobimetallic [dSdDAR10]. heterocyclic [BSDP16, CWT+12, KYKR15, LXX+10, RF15, SGHL13, WS12, dSdLB17].

heterodimer [YVT12]. Heterogeneous [DSF17, AFPI13, CKK16, YZZ+17]. Heuristic [Hel13, MS16, Tak10].

Heusler [GD10]. HeX [SLIB12]. hexa [GK15a]. hexa-aqua [GK15a].

hexabenzocoronene [RBB+12]. hexacoordinated [MC10].

Hexahalogenated [VVJ15]. hexameric [RCM+13a, RML+15].

hexopyranase [HH11, PLH16]. hexopyranose-based [HH11, PLH16]. HF [BRLS12, LGW12, MCK17a, BRLS08, Chu10, LSH+11, SKGB13]. HF/DFT [Chu10]. HF/DFT [BRLS12, BRLS08]. HFC [AR10]. HFC-263fb [AR10].
HFD [AASP18], HFD-like [AASP18], HfO [HYL+11], Hg [SLIB12, BBI+11], HGeCl [MCLd10], HgHe [BBI+11], HgXe [BBI+11], HH [LGW12], HI [LGW12], hidden [DVVP14, LTT16], Hierarchical [JYC+16, BCG10, GBFD12, KKN11, RMPAM15, SNS13], High [MCLd10, MKB+13, RSL13, BACSCJ+10, Cam15, CM13b, CSSB11, DH17, DLSd13, ESB13, EWK+13, GWPJ11, IPAA11, Jbam11, JC16, KMS16, KSM17, LL10a, MJLV14a, MO17, OPB+12, PVl+13, PVJ10, RVCFF13, REH13, SC15, WGL+11, WDLG12, ZWL13, dSAdSL13]. High-accuracy [RVCFF13], high-confidence [KSM17], High-level [MCLd10, EWK+13, KMS16, KL17, PVl+13]. High-performance [RSLS13, CSSB11, ESB13, EWK+13, LL10a], high-precision [DH17], high-pressure [WDLG12], High-quality [MKB+13], high-resolution [CM13b, JC16], high-temperature [DLDs13], high-throughput [ESB13, PVJ10], higher [NYH+17, PJ13, VKAM12, WHM10], higher-dimensional [PJ13], highlighting [BRGN12], Highly [CHG+16, HAL14, LLZA12, LwL+16, DBDP16, BkwK10a, BkwK10b, HYUS11, KOY+12, KZK+12, KV15b, OK16, TFQ+10, TJB12, LZZ14], hindrance [MP17a], Hirshfeld [Man13, VVB13, VGV+11, VBV13a]. Hirshfeld-based [OVPK15], Hirshfeld-I [Man13, VVB13, VGV+11, VBV13a]. Histidine [KFY+13, WC14], histogram [Fer17, HHWL17, SH11b, ZH12], histone [GHK12, GH10, GSD10, KC13a], HIV [DL15, Nhn16, OBW12, SYH12, TTB+10, UNT16, XLY12, ZSA10], HIV-1 [DL15, Nhn16, SYH12, TTB+10, UNT16, XLY12], HIVgp41 [AFBR17, BARM13], HMH [LDJ+10], HNcn [WHDL11], HNO [BLG10], HOB [LCL+10], hole [BSF18, Cas13, CWHH11, EPH+13, GZZM16, GA12, LZZ+15b, PAK17, PTB+15], holes [PM18], Holliday [ISH10, SHE12], holographic [CDB10], HolIT [SHE12], HOMO [RS17a], Homocysteine [AALCM11], homologated [ZLL+10], homologation [GRCL12], Homology [ZX11, BPB11, DJ13, KOY+12, XFTW15, YZZ16], homology-model [KOY+12], homology/ab [DJ13], homolysis [SZ17], homonuclear [BkwK10a, BkwK10b], homopeptides [FCD10], HomoSAR [BPC13], HONO [BLG10], HOONO [BLG11], hopping [JLH+14, KV14, LZW+11, RDR16, SRS1015], Horizontal [PC16], hormone [HYYY13, LLL+10, NS10, OME16], hormone-dependent [NS10], hormone-receptor [OME16], horsetail [MCRL17], Host [CC18b, OAN15b, YDGZ15], hot [RFHG10], Hou [JW12], HOX [LZJ+11], HP [LKL10], HP-36 [LKL10], HPT [dSDdAR10], HSE [VLK17], HSiCl [LX1], HSiCl/DSiCl [LX11], Hua [JW12], Hückel [FL15, SKT11], Huffman [QLQ11], huge [NNK+16, OHPR17], huisgen [ZZWT12], human [OME16, SLY+10, XZ11], hunter [CFM+17, SHE12], Huzinaga [Fer13b], HXEoxef [ARLP13], HXeOxeH [ARLP13], Hybrid [CR16, KS15, ...
hydroxymethylfurfural [APY+16]. hydroxynaphthaldehyde [MPSG11].
hydroxyphenylpyruvate [DGH+11]. hydroxysteroid [ZX11].
hydroxysulfanyl [TL16]. Hyper [FRN15, BLBG+13, BZB+13, RFN15].
Hypernetted [HAL14]. hyperpolarizabilities [MLC13, WYT17, YHCS11].
hyperpolarizability [ISO+13, KBC12, Lu11, TKC+11, WXS+12, WZK+13].
HZSM [cCVG+14]. HZSM-5 [cCVG+14].

identifier [Ihl12]. identifiers [GPGSM11, GPGSM12]. identify [LLHM16, LHL+10]. Identifying [AC12, HAGK10, XTY+14, LHO17, LLJ12, She12]. identity [Höf14, KN17, YN15]. IE [MLCD11]. IEF [GMMH+16]. IEF/PCM [GMMH+16]. IEF/PCM-MST [GMMH+16]. Ihlenfeldt [GPGSM12]. II [AMK11, ALH+10, ČMD13, CK17, FPB12, FB14b, GEP+14, HRJ+14, HRJ+15, JAB16, LGW12, LWXC16, 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, KT12, KTN10, KLNN10, MBC11, PPUBGD10, SOD+11, WH11, YK13, ZSYH12]. III [IKN13, KPL15, LWL+11, LXZ+10, SRL+15, BEL+11, CWT+12, GZZM16, HIS17, Zha12b, ZKH+10]. III/II [KLP15]. IKP [HLS12]. Illuminating [NSO+14]. illustrating [RML+15]. illustration [RP15]. 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, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13x, Ano13y, Ano13z, Ano14b, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s,
implicit-solvent [WWKS11]. Importance
[APA+14, CPK12, ENKK+17, NMF+14, OOK11, ESM+12, Ham11, KTNN10, PBDW11, SDZ17, TNSS17, TKNN10]. important

improve [CIKT13, DLL+10, DPSL16, Gon12, LLL+10, VLB+10]. Improved
[BS16a, LRER13, CCM15, DPB+12, DSF17, GCCM15, KSR+16, MP11, RTP+13, RDC16, SSBW14, YS10]. improvement [GSHM10, NLP+16].

Improving [CIKT13, DLL+10, DPSL16, Gon12, LLL+10, VLB+10]. Improved
[BS16a, LRER13, CCM15, DPB+12, DSF17, GCCM15, KSR+16, MP11, RTP+13, RDC16, SSBW14, YS10]. improvement [GSHM10, NLP+16].
[AMGB10, OVPK15]. intrinsically [LC16]. Introducing [DJD12].
Introduction [HIS17, Sie15, SJ17]. intuitive [EFAC13]. invariant [CWZB10]. Inverse [KTT16, GD10, JMS13, WHK+12]. inversion [SP13, GG10]. inverted [UT15, YJ17]. investigate [dSAdSL13]. investigated [SLY+10, SCW11, YS13]. Investigation [ALW+10, CAP17, GY10, PH10b, WS10, ZY14, AvKSP16, AMK11, ABB+12, ABB+13, CWT+12, CYY+17, CZH12, CH10, GDV17, HXM+16, KCB+12, KSV15b, LLM11, LLB+12, LZY+12a, LLD17, LXZ+10, MLQ+12, MP13, OAN15b, PZA15, PV12, QCR+12, RDT14, RRC+15, SH14, Tak11, TPL+10, TS10b, TR12, VVP12, YJJ+11, Yu12a, ZZ10, ZSWL12, ZBMZ15].

investigations [GZL+12, KAR12, LWWG12, TSJ+10]. Invisible [SDM+16]. involving [ARLP13, GNDA+12, LRER13, NFG+13, SLT14]. iodanes [SLT14]. iodine [ACS12, SLT14, SLT+15, YZZ+17]. Ion [Fra15, Fra16, LZTV10, DM15, DMN14, EK15, JAH+17, JTC17, KJ10, LedOLdV17, LJR+12, LPE+10, MMB+17, MH11, NC13, PYY15, PL14, RTS+13, SGS15, SV11, Tru18, TCX+13, VPR10, Vi11, WC14, ZZ10].


Ano17-27, Ano17-28, Ano17n, 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, Ano17o, Ano17n, Ano17-36, Ano17-62, Ano17-63, Ano17-64, Ano17-65, Ano17-66, Ano17-67, Ano17-38, Ano17-39, Ano17-40, Ano17-41, Ano17-42, Ano17-43, Ano17-44, Ano17-45, Ano17-46, Ano17-47, Ano17-48, Ano17-49, Ano17-50, Ano17-51, Ano17-52, Ano17-53, Ano17-54, Ano17-55, Ano17-56, Ano17-57, Ano17-58, Ano17-59, Ano17-60, Ano17-61, Ano18a, Ano18b, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h, Issue [Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18o, Ano18p, Ano18q, Ano18r, Ano18s]. Issues [GS16, MFEM16, XFG +16]. iteration [SBB10].

IV [EH13, MLGB16, VBMA13]. iVI [HLXH17, HLXH18, VHR16, ZVY +15, PGL +15].


Jumping [MS17]. junction [Ish10]. junctions [LZW +11].


Large [JBSQG11, XFG+15, XFG+16, AF14, AGR11a, CSGOA17, CHG+16, CEBO15, CSSB11, DZA11, DDM+15, FN12, GRS15, GBW+14, GP11b, GWXZ12, HLHX17, HLHX18, JS17b, KG15, KNE11a, LS11a, LCPS13, LZX16, LWL+10, LCM+14, MK11, MDT10, NYN17, NFG+13, OBP+12, RLL+10, RSL2, RSb+13, SCOJ13, SAGC16, Sch12, SRR16, SG13, SMM17, TSR+16, WLW+10, WX12, XhD15, YHCS11, ZWL13, ZLL+13]. Large-Scale [XFG+16, JBSQG11, XFG+15, DDM+15, LCM+14, MDT10, RSL+13, XhD15, ZLL+13].


WZ17, YZZ16, dRBO13, YZZ16, SHL+11. ligand-based [RVP+11].
ligand-binding [GDV17, MGWR12, OSR16, RO14b]. ligand-field [BBG*18]. ligand-induced [KL14]. ligand-receptor [FRLN10, VKC10].
ligand-sized [OGL10]. ligands [CS17, GPDC+16, HRC13, LL10b, LXZ+10, LS11b, SS+13, TS10b, ZRCC12, ZWY+10b]. ligated [EH13, WC14].
LigDockCSA [SHL+11]. light [HXM+16, KDR+18, PE11, REL17].
light-driven [HXM+16, REL17]. light-harvesting [KDR+18]. lighter [WD10].
Lightweight [RLG14]. like [AASP18, Che17, EPH+15, KOY+12, KB14b, MP17b, OAN15b, SDF+17, SM15, UCFR16, VHA+10, VVY18, WFZ+18, WKC11, WGN+16, ZSL+11, VVY18]. Limit [SN16b, Fra15, Fra16, LW16, LYC+13, OAN15a, SLT14, WTH+16].
linkage [HH11, OZS+13]. linked [Fom11, dACP12]. linked-cell [Fom11].
lists [Gon12, dACP12]. lithiated [KZK+12]. lithium [MG+10, KOP+14, KYCL11, LLL+11, MBRC16, NDG14, NFI+16, PGC12, PMT16, SKY+11, TN12, ZSL+12]. lithium-bonded [ZZL+12].
lithium-doped [PGC12]. load [Fom11]. LOBSTER [MDTD16]. Local [CHP11, GH16a, GH16b, HJKJ13, ITIN15, CPN+17, DDP16, Fer13a, HH10, KSSH13, KDS12, KGM12, Lar12, LLL+10, LZS+17, MKH+13, PH17, PRSG13, PRYI+17, PW12, SCH+12, SEF+16, WM17]. locality [Gon12].
localizability [Bar14, BLG11, BWK10a, BWK10b]. Localization [Sax12, ABDG12, BK11, BLG11, GDN+12, HIJ13, Mat14, PII17, vSGP10]. localized [Ano15-58, BH14, SB15, ZM11, dLC17]. locate [AMGB10].
Long [BCNH+11, KSH13, KSHH13, A010, BLBG+13, BZH14, JSGQ11, KB10, KV14, MMS16, MBC13, PNG10, SMGB11, ST13, SPH11, SSA+17, TSN16, VL17a, Rui11]. long-bond [KV14]. long-chain [TSM16].
Looking [WGL$^{+11}$, ZPF$^{14}$]. lookup [JMS$^{13}$]. loop
[CY$^{+10}$, FT$^{12}$, LZZ$^{14}$, NR$^{11}$, OCL$^{11}$, TJ$^{12}$]. loops [PJ$^{13}$]. loss
[GBVA$^{11}$, MH$^{11}$]. Low [BPM$^{15}$, BLDK$^{+13}$, Gra$^{15}$, AC$^{12}$, CM$^{13a}$, DH$^{14}$, LG$^{14}$, MPA$^{10}$, MP$^{12}$, MJLV$^{14a}$, RRC$^{+15}$, SN$^{15}$, SG$^{10a}$, SM$^{11}$, She$^{12}$, TF$^{15}$, TSN$^{17}$, Vor$^{10}$, YW$^{12}$, BS$^{10c}$, BBI$^{+11}$]. low-cost [TF$^{15}$].
Low-density [BBI$^{+11}$]. low-druggability [LG$^{14}$].
Low-energy [BPM$^{15}$, DH$^{14}$, MPA$^{10}$, MP$^{12}$]. low-index [RRC$^{+15}$]. low-lying [AC$^{12}$, TS$^{17}$]. Low-memory [Gra$^{15}$]. low-resolution [SM$^{11}$, Vor$^{10}$, BS$^{10c}$]. low-strain [She$^{12}$]. lowest [GFG$^{11}$]. LOX [BG$^{13}$].
LPol [BLBG$^{+13}$]. LPS [ZCS$^{+15}$]. luminescence [DBF$^{14}$]. LUMO [RS$^{17a}$]. LUMPAC [DBF$^{14}$]. lyase [CJZ$^{10}$]. lying [AC$^{12}$, TSN$^{17}$]. lysine [FHK$^{+12}$, GH$^{10}$]. lysozyme [ZP$^{13}$].
M [LD$^{+10}$, LL$^{+11}$, MCK$^{17a}$, Rab$^{12}$, TLdG$^{+12}$, WWKS$^{16}$, YW$^{12}$, YHCS$^{11}$, JJAB$^{16}$, CCCLCGR$^{014}$, MCK$^{17a}$, TLdG$^{+12}$, YHCS$^{11}$, JJAB$^{16}$]. M05 [SIG$^{+15}$]. M05-2X [SIG$^{+15}$]. M06 [LK$^{12}$]. M06-L [LK$^{16a}$]. m4 [VM$^{11}$]. m6 [Mit$^{13}$]. m6-31G [Mit$^{13}$]. machine [Aou$^{16}$, FP$^{17a}$, FSD$^{+18}$, TYZ$^{+16}$, YLCX$^{10}$]. machine-learned [FP$^{17a}$].
machines [GTZ$^{+18}$, RLL$^{+10}$, ZWL$^{13}$]. macrocycles [CMM$^{18}$, GMASBF$^{16}$]. macrocyclic [ZRCC$^{12}$]. macrolide [PG$^{15}$].
macromolecular [Kne$^{11b}$, LCA$^{17}$, LAT$^{10}$, LAT$^{11}$, PG$^{14}$, UU$^{12}$, RTP$^{+13}$].
macromolecules [DGC$^{14}$, DZA$^{11}$, FXC$^{+13}$, OHPR$^{17}$, RZ$^{16}$, ZKE$^{+17}$].
magnetic [BCSCJ$^{+13}$, BACSCJ$^{+10}$, CPRS$^{18}$, CPN$^{+17}$, FNSF$^{+11}$, GTT$^{10}$, HAI$^{+16}$, Ibr$^{17}$, JJJ$^{+16}$, XhD$^{15}$]. many-body [CGPP$^{11}$, BDdS$^{13}$, CKKK$^{16}$, HRJ$^{+14}$, HRJ$^{+15}$, JRSHP$^{14}$, KNHN$^{16}$, LY$^{+13}$, RHPWS$^{13}$, VMP$^{17}$, WCVW$^{15}$]. Many-body
[CGPP$^{11}$, HR$^{+14}$, HRJ$^{+15}$, JRSHP$^{14}$, LYC$^{+13}$, RHPWS$^{13}$, VMP$^{17}$].
many-core [KNHN$^{16}$]. map [MKM$^{+17}$]. mapper [BJP$^{15}$]. mapping [EMD$^{17}$, MMM$^{+16}$, RNSF$^{+16}$, TD$^{10}$]. maps [GJMP$^{+14}$, YSR$^{10}$]. Marburg [OLY$^{17}$]. marker [JAH$^{+17}$]. Markov [BFH$^{+13}$, LTT$^{16}$].
Mannich [AS$^{11}$]. mannose [VM$^{11}$]. Many
[CGPP$^{11}$, BDdS$^{13}$, CKKK$^{16}$, HRJ$^{+14}$, HRJ$^{+15}$, JRSHP$^{14}$, KNHN$^{16}$, LY$^{+13}$, RHPWS$^{13}$, VMP$^{17}$, WCVW$^{15}$]. Many-body
[CGPP$^{11}$, HR$^{+14}$, HRJ$^{+15}$, JRSHP$^{14}$, LYC$^{+13}$, RHPWS$^{13}$, VMP$^{17}$].
many-core [KNHN$^{16}$]. map [MKM$^{+17}$]. mapper [BJP$^{15}$]. mapping [EMD$^{17}$, MMM$^{+16}$, RNSF$^{+16}$, TD$^{10}$]. maps [GJMP$^{+14}$, YSR$^{10}$]. Marburg [OLY$^{17}$]. marker [JAH$^{+17}$]. Markov [BFH$^{+13}$, LTT$^{16}$].
Martini [HBJ$^{+17}$, SM$^{15}$]. MARTINI-like [SM$^{15}$]. mass
[NPTS$^{16}$, PGY$^{15}$]. massive [GP$^{11b}$, TNY$^{16}$]. Massively [KNHN$^{16}$, KZZ$^{+16}$, MYT$^{+14}$, BWMSM$^{10}$, KN$^{17}$, NNN$^{+16}$, OPB$^{+12}$, WHK$^{+12}$].
master [RSLS$^{13}$]. match [TZ$^{12}$, YPKB$^{12}$]. matched [KSR$^{+16}$]. matching
[AO$^{11}$, GPS$^{10}$, HS$^{12}$]. Material [JW$^{12}$, DGL$^{+13}$, HLWD$^{15}$, JBSQG$^{11}$, LL$^{13b}$, MCAG$^{+16}$, NGAS$^{17}$, SLHW$^{09}$]. materials [BSL$^{+16}$, CD$^{11}$, DLT$^{17}$, EHZW$^{17}$, EMD$^{17}$, Man$^{13}$, NDD$^{+10}$, SYZ$^{+17}$, VB$^{13a}$, VVB$^{13}$, VVY$^{17}$].
methods [Ano12u, Ano15-59, ASMS10, BG13, CLFRO18, CSGOA17, CXS10, CNK97, DKE+17, DBM+15, EWK+13, ESM+12, EV14, Fer13b, Fer13a, FB10, FSSW17, GAI14, GFPSD17, GD10, GSS13, GMO16, HCB11, HSB+11, Höf14, HWLW11, JJI+13, KSM17, KB13, KHWB17, LEoDdV17, LZLC13, LLSW14, MS13, MY17b, Mr17, MVKS10, MOS12, NYH+17, NASH15, NC13, NC14, NTNY15, OSHG17, DCO13, PN13, PVAM16, RZG+13, RRH12, SRF+17, SSB+16, SACdG14, SM+15, SGWA17, TG12b, TS15b, Tsi17, WBT10, WX12, YLCX10, YAS13, YJ17, ZGS+10, dSdLB17].
methylacetamide [HLH+12, KSK11].
methylacetylene [WCWW11].
Methylation [SCW11, KYCL11, QZM11, ALdS+15].
methylbenzyl [NDG14].
methylcobalamin [KKL+13].
methylformamides [JSW10].
methyllysine [GHK12].
methyltransferase [CPLL11, GH10, PBLdS12].
Methyluracil [HvM17, HvM16].
MetREx [Sti15].
metric [CXS10, LLFH16, PKIC11, SOJ14, ZT14]. metrics [Hug14, PBBP11, RCM+13b].
Metropolis [MO15, Pon10].
Mezev [HJJ13].
MF [YKH15].
Mg [LDJ+10, BMFG16, DOM+11, PLZ17, PYY15, RRF11, SS13c, ZZ10]. Mg-porphyrin-based [PLZ17].
MHC [HHWL17].
MIA-QSAR [BF15].
MICPB [CCC+11].
micelles [WWKS11].
Michael [NDG14].
microbes [RSLS13]. microclusters [NC12].
microelectrostatic [SM17b].
microhydrated [SM17, ZYP+15].
microhydration [OSS10, SB+17]. microiteration [SMM17].
microiterative [RR12].
micromolecular [XTG+11]. microscopic [HLWD15].
microscopy [LLJ12].
Microsecond [DMN14]. microseconds [Bow16].
microstructures [DASA15].
microwave [BLF14].
MIDAS [GJMPA+14].
Midpoint [JMS14].
migration [FBEM11, Ish10, KYKR15, RSB+13, TN10].
milestoning [BRE16].
mimetic [MV17].
mimic [GRP+12, ZWS+10].
mineral [TJZ11].
mini [CFC15, HTS15, HtS17].
mini-protein [CFC15, HTS15].
mini-proteins [HTS17].
minima [AC12, GFG11, HvM12, SGWA17].
minimal [CGBK13, CG12, OYK+11, RSR+12, RVVK13, WHAS+10, WHAS+16].
minimization [GBVA11, RAO11, TJBI12, XHLH16].
minimized [ZAZ].
minimizing [KS12].
Minimum [RAR+11, CY09, CY13, LLSW14, MP13, MCAY15, PRP15, PHDH13, SRSLO15, SG10b, Tak10].
mixing [BCP+10, MDC12].
miniprotein [MTD10].
minnesota [LH14a].
minnesota-type [LH14a].
minnow [TTL+12]. misfolding [LH11].
mismatched [BH13].
mispair [BZH14].
Mixed [RdA12, BRGN12, BEEL14, BACSCJ+10, DH11, DFF+15, Fer13b, Fer13a, GMASBF16, GG10, Ibr17, KGR+16, LYL16, MP13, PSdcP+10, RB12, TS10b, VVJ15, WX12, YLL11].


Modern [AB16a, AB16b, DH17, Fon11, LMR14, SDM+16]. modes [CBP+15, GMPB12, LLTC12, MS17, dSaSL13].

Modern [AB16a, AB16b, DH17, Fon11, LMR14, SDM+16]. modes [CBP+15, GMPB12, LLTC12, MS17, dSaSL13].

Modern [AB16a, AB16b, DH17, Fon11, LMR14, SDM+16]. modes [CBP+15, GMPB12, LLTC12, MS17, dSaSL13].

Modern [AB16a, AB16b, DH17, Fon11, LMR14, SDM+16]. modes [CBP+15, GMPB12, LLTC12, MS17, dSaSL13].

Modern [AB16a, AB16b, DH17, Fon11, LMR14, SDM+16]. modes [CBP+15, GMPB12, LLTC12, MS17, dSaSL13].

Modern [AB16a, AB16b, DH17, Fon11, LMR14, SDM+16]. modes [CBP+15, GMPB12, LLTC12, MS17, dSaSL13].

Modern [AB16a, AB16b, DH17, Fon11, LMR14, SDM+16]. modes [CBP+15, GMPB12, LLTC12, MS17, dSaSL13].

Modern [AB16a, AB16b, DH17, Fon11, LMR14, SDM+16]. modes [CBP+15, GMPB12, LLTC12, MS17, dSaSL13].

Modern [AB16a, AB16b, DH17, Fon11, LMR14, SDM+16]. modes [CBP+15, GMPB12, LLTC12, MS17, dSaSL13].
[Ano12u, MIS+15]. modified [BD12, CH16, DPSL16, DJX+11b, GSD10, MRO17, Mit+13, SMM15a, SMM15b, SMM+18, XYX17, XVA+16, ZZ12].


modulation [PE11, RS17a]. modulator [ILKR11]. modulators [SRA17].

module [PHH+12, VBV13b]. MOFs [LPK16]. moieties [SPL+18].

MOLCAS [ADF+10, VBV13b, AAC+16]. Moldyn [HPSK12]. Molecular [AAStP18, BDTP11, BSF18, CRZ+18, CMD13, Cor17, DGH+11, DHF+11, DSX+11, Fom13, Ibr11, KUDG12, KB14a, LWZK13, LDPM12, MFEM16, PL14, Pla11, RKG10, RO14a, RKK14, Sch18, SBT17, SFLG+17, SV11, VSD10, WC11, WWKS11, XFG+16, XLY12, Yan16, YJXZ13, ZWS+10, AALCM11, AG11, ASL+11, AS10, APK14, AGB13, AS15b, AGR11b, AJR16, AB16a, ASK18, ALH+10, BMR11, BAMR13, BE16, BSI12, BV14, BW15, BJF17, BIP15, BMBJ11, BE16, BV13, BE+11, CBP14, CMM18, CM13a, CDBM11, CD13, Car14, CTR13, CAF+13, CEB10, CIKT13, CGPP11, CS14, CXW4, CBTZ16, CH16, CCOH14, CVG14, CCW+10, CHK10, CB11b, CB11c, CM16, DJM17, DSD+11, DJX+11b, DLZ15, DPD+15, DL16, EP10, EK15, EJ13, EPF+13, ENKK+17]. molecular [EPD+11, FBEM11, FSC+14, GBL+11, GDV17, Gar12, GJMPAM+14, GSHM10, GR11, GMZ12, GMMH+16, FFGS18, GLY10, GWZ15, GCV14, GGM+12, GBW+14, GEP+14, GPdC+16, GP11b, GR10b, GPK12, EPF+15, HS17b, HB14, HS12, HCD+10, HDM+15, HSK12, HH16b, HWLW11, HJ10, HX+16, HHWL17, HRI16, HC14, IUK+11, IIF+10, IM17, IU10, JS13, JBSQG11, JAH+17, JSXH16, JWST10, JGS+17, Jor17, JMS14, JS17b, JP15, KCK+17, KCK+15, KVQC+11, KGHK12, KGC+15, KL12, KJD12, KDB13, KERY+16, KTSW11, KLOS10, KJM+17, KC14, Kos16, KSR+16, KG13, Kow11, KTN10, KV15a, KVR10, KSW16, LPAS11, LL15, Lar12, LWK+14, LGBS16, LH11, LL13a, LJ12, LFN+10, LLC+10, LL11, LZY+12a, LMI+14, LAHS16, LPE+10, LLTC12, LCB10, LZW+11, LTP11, LZL+13, LWXC16, LZS+17, LJL+11, LP11c, LAS+14, MRB14, MKS+12, MSC+10, MJC14, MCRL17]. molecular [Mat10, Mat14, MSvG12, MJW+11, MFEM15, MADWB11, MPNS13, MMK+17, MBA14, MRHR11, MCC12, MFR+17, MO17, MS12, NPTS16, NSF+14, NLB+16, NST14, NPG17, NFPD13, NFG+13, NF17, NPK+16, NHK+13, NS17, NTRY15, Oh16, ONHK11, ON14, OGL10, OHR17, OCL11, OLY17, OT12, OME16, OVPK15, OOT15, OCW+15, OZS+13, OOK11, PMC+17, PSS14, PAK15, PAK17, PH17, PSG+17, PM13, PGW+17, PVZ13, PJ13, PBG17, PS10, PVAM16, PLP+16, Pro16, PH15, PVJ10, RMPAM15, RLLH12, RNSF+16, RPG13, RNP13, RS12, Ras17, RHJ11, RO14b, RR14, RLG14, RSR15, REH13, SHMO11, SLT+15, Sax12, SVM10, SK15b, SA13, SZTSM10, Sch12, SFN+11, SHF11, SMRM+17, SOM+13, SJ17, SR18, SYN+12, SK13, SWB+12, SLL13, SJ16, SDMS13, SKY+11, SBvG14, SAvG15, TNYN16, TKNN10, TZ12, US11]. molecular
multi-core [KK17a]. multi-fragment [VBV13b]. Multi-level [FFA14].
multi-nanosecond [MCRL17]. multi-objective [PSG+17].
[CXW14]. multilevel [TNY16]. multiline [GJMPAM+14].
multimolecular [CD16]. Multiobjective [BDdS13]. Multiparticle
[NDW15]. multiphase [BVY+12]. Multiple [JS17b, LL10b, YZ17, AYYO17, CD11, CL16, DGC14, DSX+11, ESB13, FBEM11, GA12, KJM+17, LZY12b, Rob13, RFHG10, TNSS17, YDX16, PPUBGD10]. multipliers
[GREA11, RHJ11]. multiply [RJS17]. Multipolar
[YMP14, FCCP17, HCP15, KFY+13, KWL+16, NLP+16]. Multipole
[NOKJ16, SWPR11, BLDK+13, CP15, CTP13, EPD+10, EPD+11, Kan15, KR12, KSK11, Lar11, LBGS16, SLX+15, Tru18]. multipoles
[Elk16, KGM12, SMP17b]. multiprocess [MB16]. multiprocessing
[GP11b]. Multireference
[GA14, SP13, CCM15, CF14, GCCM15, MCC11, MC12, SSSM15].
multiresolved [DGC14]. Multiscale
[BLKP12, FXC+13, LC16, LZ14, JBB+11, MBC13, SYN+12, WLO+17].
multisite [CK17, HS14b, MMB+17]. multistart [MS16]. Multistate
[TM16, AM10]. Multistep [DWZ+17, FZY+12, WDZN16]. Multistructural
[SMM17]. Multisubstrate [PBLdS12]. multithreading [TO10, ZWL13].
multivalent [AS14, FVP14]. Multiwfn [LC12]. Mus [WZQW10].
muscarinic [TRA17]. musculus [WZQW10]. mutagenic [BZH14]. mutant
[FHK+12, LMA15]. Mutantelec [VRMSH+17]. mutants [RKDM14].
mutation [BA11, VRMSH+17, ZJZM13]. mutations
[BH15, GNO16, KYT+17, SL10, SY16a, WC11]. mutual [BMPML+13].
MVPACK [BACSCJ+10]. MX [Sch13]. mycobacterium [MPNS13].
MyMolDB [XTG+11]. myoglobin [SHB17].
PVL$^{+13}$, BCNH$^{+11}$, BWKW$^{10b}$, BMB$^{13}$, BSDP$^{16}$, CWT$^{+12}$, CCM$^{15}$, DCHL$^{12}$, DLW$^{12}$, GMASBF$^{16}$, GZL$^{+12}$, HLH$^{+12}$, KV$^{14}$, KCL$^{+14}$, LZL$^{+15b}$, MLGB$^{16}$, MS$^{15}$, OZLSBH$^{12}$, PVL$^{+13}$, RHNN$^{10}$, RWR$^{+13}$, ŠBD$^{+17}$, SGHL$^{13}$, TSJ$^{+10}$, VM$^{11}$, WS$^{10}$, WGL$^{+11}$, WCL$^{+11}$, WYGW$^{12}$, WS$^{12}$, Yu$^{12b}$, YXZZ$^{17}$, ZP$^{13}$, HPSK$^{12}$, N- [BMB$^{13}$], N-heterocyclic [GZL$^{+12}$], N-methyl-N-phenyl-hydrazine [BSDP$^{16}$, CWT$^{+12}$, SGHL$^{13}$, WS$^{12}$], N-methylacetamide [HLH$^{+12}$], N-substituted [DCHL$^{12}$], NABs [SBW$^{12}$, SBW$^{12}$], NABs-Li [SBW$^{12}$], NaI [OCW$^{+15}$], NaIyang [Ano$^{12u}$], nano [Ano$^{15-58}$, BH$^{14}$, QZ$^{10b}$], nano-clusters [QZ$^{10b}$], nanobiotechnology [Fe$^{10}$], nanochannels [TM$^{16}$], nanocluster [AS$^{15a}$, RVK$^{13}$], nanocusters [AASP$^{18}$, LLJ$^{12}$], nanocluster [AS$^{15a}$, RVVK$^{13}$], nanoclusters [AASP$^{18}$, LLJ$^{12}$], nanocrystal [KC$^{13b}$], nanographene [DW$^{+17}$], nanographenes [TSN$^{17}$], nanolayers [EBK$^{13}$], nanoparticles [CCJC$^{10}$, NNS$^{15}$], nanoparticle-PMMA [NNS$^{15}$], nanoparticles [EOO$^{+16}$, LZZ$^{+11}$], nanopore [SM$^{16b}$], nanopores [DMN$^{14}$, MJC$^{14}$, SM$^{15}$], nanoribbon [DJX$^{+11b}$, DJX$^{+11a}$, RRK$^{14}$], nanoribbon-based [DJX$^{+11b}$, DJX$^{+11a}$], nanoribbons [WZK$^{13}$], nanorings [TS$^{15b}$, YDGZ$^{15}$], nanorods [LHKS$^{12}$, LH$^{14b}$], nanoscale [Hei$^{10}$, SWB$^{+12}$], nanosecond [Bow$^{16}$, MCRL$^{17}$], nanosheets [wZb$^{11}$], nanosheet [wZ$^{11}$], nanosheets [TSN$^{17}$], nanosystems [Tia$^{12}$], nanotube [AS$^{15a}$, FTR$^{15}$, JWO$^{15}$, RHNN$^{10}$], nanotubes [AS$^{15a}$, FTR$^{15}$, JWO$^{15}$, OCW$^{+15}$, RHNN$^{10}$], nanowires [EP$^{15}$], naphthalenediimides [MGS$^{+16}$], naphtho [ZLL$^{+10}$], naphthalenediimidines [MGS$^{+16}$], naphtho [ZLL$^{+10}$], naphtho-homologated [ZLL$^{+10}$], naphthodithiophene [MGS$^{+16}$], naphtoid [CYY$^{+17}$, GZL$^{+12}$], native [DJ$^{13}$, HYL$^{+11}$, UCFR$^{16}$, YL$^{13}$], native-like [UCFR$^{16}$], Natural [LCPS$^{13}$, MBFP$^{15}$, Wei$^{12a}$, Wei$^{12b}$, AO$^{10}$, GMZ$^{12}$, NC$^{14}$, Sch$^{12}$, GLW$^{13a}$, GLW$^{13b}$], naturally [XVA$^{+16}$], Nature [ABDGN$^{12}$, MJ$^{+15}$, OC$^{+15}$, WY$^{15}$, YZN$^{13}$], network [MS$^{15}$, PPUBGD$^{10}$, RKDM$^{14}$, WMW$^{+10}$], network-based [OC$^{+14}$, PPUBGD$^{10}$], networks [AG$^{+13}$, Clo$^{15}$, Kan$^{15}$, KUDG$^{12}$, LHO$^{17}$, PPM$^{15}$, PPUBGD$^{10}$, TD$^{11}$], neural [AG$^{+13}$, HNHR$^{13}$, LHO$^{17}$, LD$^{+14}$, PC$^{+11}$, PPUBGD$^{10}$, RKDM$^{14}$, WMW$^{+10}$], neutral [GC$^{11}$, GWP$^{+11}$, JM$^{+11}$, KD$^{10}$, Ts$^{14}$], new-type [HLWD$^{15}$], News [AIGP$^{15}$, Aki$^{16}$, APK$^{14}$, AAC$^{+16}$, BTA$^{+13}$, BHB$^{+12}$, BCSCJ$^{+13}$, BSZ$^{+12}$, ...
optimization-based [YS15], optimizations [RR12, WX12], optimized [Boz18, CX10, GA12, HH10, LZZ14, NDW15, ŠŠB+16, SB14, WO15].


Orbital [WM12, ASL+11, Boz18, BVC13, CIKT13, CPN+17, CGPP11, DHF+11, FE14, GWF11, GLW13a, GLW13b, IIF+10, IKN13, KTNN10, LCPs13, LFN+10, LTP11, MFR+17, MGS+16, NF17, OHNK11, OOT15, OOK11, PRY+17, PH15, RKGN10, SGPJS+17, Sch12, SSMMW09, SB14, SB15, TKNN10, TS14, TSN16, US11, UM13, Wei12a, Wei12b, WCWV15, WM17, ZA15, vLBRR12].


ordering [LPAS11, LC17a, LLB+12, SJZ+15]. ordering [MNNK10a, MNNK10b].


overestimation [FHK+12]. overlap [BBG+18, SFDE16]. overlapping
generalized [HWLW11]. GIAO-CCSD [OPR16]. GULP [SN16a].
Hamiltonian [KCK+17]. hydride [PM13]. hydrophilic [PAK15]. II
[HYUS11]. MC-XQDPT2 [KKL+13]. metal [BS16]. MgO [BS16b]. MM
[BM12, AALCM11, BTA+13, CZY11, CJZS10, DSK17, DSX+11, FLM11,
FPB12, FB14b, GWZ15, GCW14, HH15, HBR17, JHH+13, JWS10,
KTN10, KWL+16, KWG15, LFM12, LT13, LHT15, LLL+11, MCRL17,
MTG12, MJG+15, NO16, PMC+17, PDMT10, PL14, RR14, RN17, RR12,
SN16a, SGDT10, SJ14, SCM+15, STM+15, SSAS10, TSC+13, VKNT15,
VKNT16, VCM15, VKTRJ15, WDP+12]. MM-MD [RSR+12, OYK+11].
MM-QMC [UTM11]. molecular
[BEL+11, Fer13b, Fer13a, Rad12, YK+11]. multiple [JS17b]. NaCl
[HB15]. nucleobases [CC11]. nucleophilicity [TMJ15]. OD [Chu10].
oligomerization [KAR12]. OpenMP [KS15, KN17]. or [KB10, Pog10]. PB
[GMMH+16]. phenol [LYK11]. phosphorus [GW+12]. Poisson
repulsive [SNK16]. SAC-Cl [EFS16, IN13]. Si [LGKS17]. superoxo
[ZRC12]. TD [TS15b]. TD-DFT [LXZ+10]. TDDFT [MS11]. thymine
[HvM12]. time-dependent [JYS+12]. TIP3P [SC10]. uracil [HvM12].
vacancies [HRB+17]. Vis [GGM+12]. water [JA10, SV11]. X [BS18]. Zn
[GE+14]. penetration [NLP+16]. Pentaatomic [Xb15]. pentacene
[CWHH11, YG+15]. pentacoordinated [TS10]. pentagon
[Fl15, GZH10]. pentane [TCGNT18]. pentaprismane [PCL11].
pentathienoacene [YG+15]. penten [LXFC17]. peptide
[FP17a, HPL13, HLH+12, ICS+12, ICS+13, JBAM11, JWS10, LTT16,
LW11, LLvG10, LJW+11b, Lvg13a, LMA15, MDT10, MV17, OZ14, QZM11,
SV15, SEM12, TYZ+16, XHLH16, YZ15a, dCLFGL13]. peptide-backbone
[HLH+12]. peptide-design [XHLH16]. peptides [BLKP12, BPC13,
COCH4, CZN11, CFG11, HLH+12, HHW17, IO13b, JXC10, KB10,
Lvg13c, MZZ11, OLY17, WNM17, XHLH16, XWS13, ZKH+10]. peptoid
[MMZW14]. perception [AJ16]. HYZZ13]. Performance
[Abr11, BZB+13, CSKH16, CKK16, DOM+11, GJIR18, HS+11, JCP14,
KL16a, KRB+14, SGW17A, ABM+15, BLBG+13, CLFR018, CXS10, CSSB11,
CJZS10, ESBI3, EWH+13, GA14, GRARO+14, GSS13, HWL11, KZZ+16,
Ll10a, LRB12, LLC+10, MHT+18, MC12, MG11, OPB+12, RRH12,
RSL13, SRF+17, SPR+13, SJ16, TF15, YPC+10, ZSL17, ZWL13, SBW12].
Pericyclic [HPT16a, KG15]. Periodic
[Sce07, Sch10, AAC+16, CMM18, CEBO15, FCD10, Gar12, HSH15, HHI+17,
ITIN15, KB14a, LBGS16, Man13, MGS+16, NN18, NO16, NNTN15, RJPB12,
SN16a, Ste15, TLG+12, Tak14, VB13a, VB13b, VECT12, VI17]. Perlin
[HLBLCCG15]. permeation [DMN15]. permutation [AO13b]. pernitrides
[WD10]. perovskite [LLB+12, LLL+12, VY17]. peroxide
[KNP+12, MK13b, SZ17]. peroxy [RHPWS13, RHT+15, ZRC12]. peroxy/
superoxo [ZRCC12]. peroxynitrous [BLG11]. persistence [XW15].
Persistent [XFTW15]. perspective [ABDGN12, Dil15, Hsu14,
JCGVPH17, JM+16, LGOM+15, MP17a, Niz13, PZM15, XLY12].
perspectives [DR14, Wei12a]. perturbation
[CCM15, CF14, DCHL12, FRSA14, FSSW17, FE14, GRS15, GCCM15, Hil13,
HRJ+14, HRJ+15, HYUS11, JRSHP14, KKNN11, KN17, KM13, LCL+10,
LlvG10, LGL11, Lg13b, Lg13a, MCC11, RLDJ17, RAR+11, RHPWS13,
SSM15, TAG16, VDL+13, WHAS+10, YKH15, ZZ14, WHAS+16].
perturbation-selection [FE14]. perturbations
[GMSdG15, OSR16, Tak10, WWCL15]. Perturbative [SSWX14].
perylene [BSL+16, SLP+12]. perylene-based [SLP+12]. perylenediimides [QCR12].
pesticide [BHB+17]. peta [KNHN16]. peta-scale [KNHN16]. petascale
[SCOJ13, ZWL13]. PH [LZL+15b, dSDdAR10, LZL+15b, AB16a, CS14,
CAD16, HS14b, MBA14, PS13, SY16a, SOvG12, Vor12].
pH-dependent [SY16a]. pH-responsive [MBA14]. Phage [MP17b].
Phage-like [MP17b]. PHAISTOS [BFH+13]. pharmacokinetics
[VBDS+11]. Pharmacophore [HRK+10, HKRS11, HS11, TD10, AKMT11].
Phase [ATM18, ZWMW10, ABB+12, BE12, BG17, DLSD13, DLW12, EMD17,
GYX+10, Hsu14, KD10, LJW11a, LPLB16, LGKS17, MFM+12, NIIT15,
PSC11, RWI+13, RSLML12, RJS17, SJZ+15, VKAM12, VED10, YHG+11,
YS12, ZS+14, ZWW10, ZYR+15, ZLHH14, dSDs12a, dSDs12b, ABB+13].
phase-change [EMD17]. phases [EB12, LPAS11]. Phen [FD16]. phenol
[AAMD+11, AK10, PPH+14, WHX+10, YKH+10, AK10].
phenol-imidazole-base [YKH+10]. phenol-triethylgermanium
[WHX+10]. phenolates [SKGB13]. phenols [SK12]. phenomena
phenyl [GZL+12, ZWY+10a]. phenylacetylene [ZZL+12].
phenylacetylene-containing [ZZL+12]. phenylalanine [GWF11, PV11].
phenylaziridines [KYL11]. phenylene [CH10]. phenylhydrazine
phosphaalkene [TR12]. phosphano [KYR15]. phosphate
[MRO17, XZ11, YZS14a]. phosphatidylcholine [PVM10]. phosphatene
[SHL+13]. phosphine [MG14, YK13]. phospholipid
[PS10, RBOH11, SDZ17, WLO+17]. phospholipid/cholesterol [RBOH11].
phosphopeptide [AC11a]. phosphoranes [TR12]. phosphorescence
[LW+11, LXZ+10]. phosphoric [HPT16a]. phosphorous [KLN12].
phosphorus [RB12, YDX16]. phosphorus-containing [YDX16].
phosphorylation [RIJ+11]. Photo [HNN+17]. photochemical [Su10].
photocycloaddition [LXFC17]. Photodeactivation [Ant13].
photodetachment [MLCD11]. photodetectors [DPAB16]. photodynamic
[ZZ12]. photoelectron [FF11, MLCD11]. photoemission [RJS17].
photoexcitation [RVDMB16]. photoexcited [MS11]. photoinduced
[CGP12, MSV16]. photoionization [MY17a, MY17b]. photoisomerization
FBEM11, HTS17, JM11, KV15b, LPLB16, PAK17, PTB15, REL17.

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[TLdG+12, CK17, NJX+10, PKK17, PGdO+16, YDR13]. **Pt-195**

[PGaO+16]. **Pt-based** [NJX+10]. **PTCDa** [HB15]. **PTCDa/KCl** [HB15].

**PTCDa/NaCl** [HB15]. Pteros [Yes12, Yes15]. Published

[GS16, MFEM16, XFG+16, Ano12u]. Puigjané [Ihl12]. pull [MLQ+12].

**PUPIL** [BTT10]. pure [BG13, LBH+11, SN15]. purely [BDdS13, purine


**PyADF** [JBB+11]. PyFREC [KDR+18, Kos16]. PyGlobal [NkJ16]. PyMOL

[BTA+13, HL14]. PyMOL360 [HH16b]. PyMOL360 [HH16b].

**PyMOL** [BTA+13, HL14]. PyMOL360 [HH16b]. pyMolDyn [HRB+17].

**PYP** [UD12]. PyPES [SC15]. pyramidalization [Gav12]. pyrazine [WDP+12].

PyRETIS [LRvE17]. pyridin [BMB13]. pyridin-2-yl [BMB13]. pyridine

[LWL+11, MFR+11, PMC+17, SLLL13, YLZ+10, CCLP12]. pyridone

[AFSW16]. pyrimidin [YZ15b]. pyrimidin-4 [YZ15b]. pyrolysis


Pyruvate [CJZS10]. Python [HPT+16b, LRvE17, PHH+12, Yes15].

**PYX** [LWWG12].
quadrupolar [CSEMB+16]. quadrupole [HBKL10, LIRL+16].
quadrupoles [NLP+16]. Qualitative [YK13]. Quality
[CLK11, KCK+17, KYB13, MKB+13, POB13, RB13a, RCM+13b, SC15].
QuanPol [TSC+13]. quantification [Hamb11, PC14, YNH+17].
quantify [LLHM16]. Quantifying [TMJ15, GMBX+16, MS10].
Quantitative [DZA11, RDT14, V˚AA14, Wei12b, BPC13, CD13, DKL+10, NFG+13, REL17, RCM+13b, XFTW15, TTB+11]. Quantum
[ALK+15, AC11a, APA+14, Cha10, CG12, DDM+15, FRN15, GH10, HHDC16, KASH14, Li14a, Li14b, LWD13, MBRC16, MS12, RFN15, SC0J13, SAGC16, SBD+17, SOY12, SR10, SHB17, TR12, UD12, WCAH10, WDP+12, Aki16, ASS+17, ARAG17, AAC+16, APY+16, ACS12, ASK18, ALH+10, Bac12, BTT10, BRP+12, BGR13, BEL+11, Cam15, CBH14, CDM10, CDB10, CDBM11, CD13, CD16, CXW14, CHK10, CM16, DR11, DKT13, DPAB16, ECZW17, EV14, Fer13b, Fer13a, FFB10, FLM11, GPM17, GMMH+16, GTK10, GGM+12, HZ11, HLvdV13, HPT+16b, HGCCGR+16, HMM10, HYUS11, HGY15, JBB+11, JSXH16, KP11, KVR10, LPE+10, Lü14, MP17a, MAP10, MSvG12, ME10, MSSP17, MHH11, MFR+11, NC13, NC14, NNK+16, NDD+10, NHK+13, NS17, OKIS17, OSM16, PML+12, PSC11, PGW+17, PG17, PVAM16, RLLHL12].
quantum [REL+14, SLT14, SS13b, VPR10, VBMA13, WKC+10b, WBT10, WAB17, YKO+11, YW13, YHK15, ZW17, ZVY+15, dCDP15, BLG10]. Quantum-chemical [KASH14, FB10, MSvG12, MFR+11].
Quantum-chemistry [DDM+15]. quantum-classical [HLvdV13].
Quantum-mechanical [ACS12, ECZW17, PGW+17]. quasiclassical
[Cha10, LWD13, dSVdM+16]. QuBiLS [JMPAM+14]. quest
[AOW11, EK17]. question [BZH14]. quick [VVV+15b]. QuickFF
[HRJ+14, HGHP14, HR+15, JRSHP14]. quinolone [ZCK+16]. quinone
[GLM+17, VSD10]. quinones [uLhY11].
R [LdSRR16, NDG14, Sch10, LdSRR16]. R-C [LdSRR16]. R-Group
radiation-damaged [LZH+11].
radiation [LZH+11].
radiation-damaged [LZH+11].
radiation [LZH+11].
radiation-damaged [LZH+11].
radiation [LZH+11].
radiation-damaged [LZH+11].
radiation [LZH+11].
radiation-damaged [LZH+11].
radical [AAMD+11, GAI14, GKR13, JCG+10, KGR+16, KV14, LJJ+11, Ray13, RKG11, SJD11, TTR+12, TL16, WHDL11, ZZZ+10b, ZLZ14, ZSZ+14, dLC17].
radical-bridged [ZLZ14]. radical-formic [TL16]. radical-molecule
[GAI14]. radicals [Den12, KS13b, SRR16, WCT+11, WLHZ12, ZZZ+10a].
radii [STM+15, YMT14]. radio [AB10]. Rugué [Ano16-56].
Ramachandran [KS12, MP17a]. Raman [PAK15, SLLL13, YB13].
Random
[HMM10, AC11b, CY09, CY13, CLK11, GPM17, OLA15, RDRC16, WZ17].
Randomized [JPC11]. range [AO10, BLBG+13, BCNH+11, BK17b, CSKH15, HH15, HZSS17, Jan16, KB10, KSH13, KSSH13, MMS16, NLP+16, RSG14, Rui11, SMGB11, ST13, SPI11, SZZS16, SSA+17, VLT17a, WYT17].
Reoptimized [HLH+12, HH11]. reorganization [BE16, DAdGR15, RJS17].
Reparameterizations [DPJ16]. reparametrization [DH11, FCE15].
replacement [YHW17]. Replacing [ZSB+16]. Replica
GS15, GS16, XFG+16, ZC14, CH16, CCOH14, IO13a, IO13b, KCK+17,
KTO11, KTO13, LC17a, LMI+14, MS16, OGL10, OL13, OLY17, OZ14,
RFHG10, SBN13a, SBN13b, TKT11, XFG+15]. replica-exchange
[CCOH14, IO13a, KTO11, KTO13, LMI+14, OLY17, OZ14, SBN13a, SBN13b].
replica-permutation [IO13b]. replicas [LL11]. Reply
[Can11, Cor17, GKR13, QB11, VVB13, WM12, LAT11]. representation
CXW14, CWZ10, FXC+13, HZY+10, KCPMG12, KDS17, LLLC11, ME10,
YDL+10, YS10, YHH+13]. representations [OVPK15, dVZ17].
representative [KV12, KV13, VLGK+17]. representing [TY10]. repressor
[OHNK11]. reproduced [Zha12b]. reproducibility
[GKR13, Ray13, RKG11]. reproducing [KTNN10, MAK+14]. reproduction
[OPBR17]. repulsion [BOB16, CGPP11, ENKK+17, HOK17, PS17, PC16].
repulsions [JJH+13]. repulsive [IO13a]. required [RAR+11, SG10b].
requirement [BF15]. requirements [TS15a]. requires [Bow16].
resampling [MMM+16]. rescaling [LL10a]. rescoring [BMR11].
LABSG17, BH15, BA11, GMO16, IHIY15, NR11, SL10, SEF+16, WC14,
YHH+13]. Residue-centric [LABSG17]. residues
[FKH+12, KLS10, KMLS10, RKDM14, SK17, WX1+12, WC14]. resistivity
[AB10]. resolution [BMFG16, BS10c, CM13b, DFF+15, Höf14, JC16, KN17,
NPG17, SM11, VOR10, WNM17, YN15]. resolution-of-identity [YN15].
Resolutions [LMR14]. resolving [AVHB18]. resonance
EF16, KN+12, YB13]. resource [Gil11]. Response
[GPGSM12, dSdS12b, BZH14, DHE+12, ESM+12, ITIN15, KSSH13,
KZK+12, LP11b, MRB14, RJR14, RCM+13b, SS16a, SDF+17, WGLG+16].
responses [GWX+12, MLQ+12]. responsive [MA14]. restrained
[HCD+10, KCK+17, SR18, ZDZM13]. restraining [KOY+12]. restraint
[RO14a]. restraints [SM11]. Restricted [SL10, Cas13, PDG+16, YD17].
restriction [FSD+18]. result [PH15]. results [Ber17, CBH14, CLK11,
GR10a, KERY+16, PLAG11, RAR+11, SHL+13, WDHZ13, KMLS10].
retinal [CG12, SGWA17, ZLHH14]. retinoic [LMF12]. Retracted
[ANO12a, GRL+12]. retro [GRCL12]. retro-imo-ene [GRCL12]. reveal
[MA16, RKDM14]. revealed [ALH+10, PNG10, VKN15, YZGS14b].
Revealing [VVY17, YW13, YJ17, Bac12, GFGS18]. reveals [NR11, WC11].
Reverse [LWL+16, ASL+11, Aou16, GP12, OPBR17]. reversible [RII+11].
Review [DR14, FRSA14, GHV17, JCL+17, CMVg10, Sch10, Spr10].
Reviews [HLvdV13, ZW12]. Revised [AKMYB18]. Revising [Pla11].
Revision [PLH16]. Revisited
[KR14, ASS+17, CYT+10, Dii15, HZ11, HFSO12, MSBF16, YW13, vSGP10].

LCL$^+$10, LPS$^+$13, MLQ$^+$12, yOTn16, ŠSB$^+$16, TAG16, WYT17. Second-
[TKN13]. Second-order [MCC11, DCHL12, Hil13, KKNN11, KN17, LCL$^+$10, MLQ$^+$12, yOTn16, ŠSB$^+$16, TAG16]. secondary
[Clo15, DWL11, FZY$^+$12, HNHR13, HTS17, KT10, KS12, LFB14, LGL11, Man14, QZM11, SM11]. secretase [YLCX10], secretory [FZL$^+$15]. section
[HBL12, dCLFGL13]. selections [MY17a, MY17b]. SEDD [HNN$^+$17]. Seebeck [FSD$^+$18]. Segmentation [TSR$^+$16, LCM16]. segments
[yOaCG10]. selected
[ICS$^+$12, ICS$^+$13, KCL$^+$14, SGM$^+$13, VSD10, dSAdSL13]. selection
[FE14, HS17a, HS17b, KDB13, WMW$^+$10, ZYS$^+$10]. selections [HYMZ16].
Selective [PXXW10, LZZT10]. Selectivity [LPLB16, dSdLBNB17].
[AFSW16, CD11]. self-assembly [Hei10, KN16, uLhY11]. Self-consistent
[JSXH16, BK17b, DK11, GBVA11, HKR$^+$14, IM17, KC13b, KT10, KLN16, MJLV14a, ON14, OCL11, SPS$^+$12, SCSW13, TYN15, WMW$^+$10, YN15, uLhY11].
[HS17a]. self-metathesis [MJLV14a]. semi [FSSW17, SC15]. semi-direct
[FSSW17], semi-global [SC15]. semiconducting [VS14, ZL17].
semiconductor [LCH$^+$15, SFDE16]. semiconductors [BE16, NDLW13].
Semiempirical [SRL$^+$15, GP11a, HGY15, KTN10, KB14b, LSD$^+$10, MGWR12, SPH11, SDL14, TKN10, TG12a, UCWR16, WCWV15].
semiexperimental [VDVR14]. Seminumerical [PW12]. sense
[DR14, ICS$^+$12, ICS$^+$13]. sensing [LZL$^+$10, RRK14]. Sensitivity
[Han11, LL11, LWG12, PDG$^+$16, Sea10]. sensitized
[ACS12, JYS$^+$12, LZL$^+$15a, YJN$^+$11]. sensitizer [YJN$^+$11]. sensitizers
[SQC$^+$17]. sensors [DHE$^+$12]. separable [WWU12]. separated
[BK17b, HZSS17, RSG14, SZS16, WYT17]. separation
[CSKH15, DS12a, VL17b, YSG12]. Sequence [TYZ$^+$16, DLL$^+$10, DWL11, LXL$^+$11, MP17b, Sti15, WXL$^+$12, YZWC11, YS10, ZWP11, HYMZ16].
Sequence-based [TYZ$^+$16, WXL$^+$12]. sequence-reactivity [Sti15].
Sequence-specific [HYMZ16]. sequences [Ano12u, CCYL11, Fel10, HZY$^+$10, LMZ$^+$11b, LLLC11, LDH$^+$14, OLA15, QLOQ11, YDL$^+$10].
Sequential [CBP14]. Ser [LY10]. serial [BB11a]. series
[AC11b, DDM$^+$15, LZGS11, MCK17b, SRA17, SB10, TD10]. serious
services [LP11a, UHH$^+$11]. Set
[SN16b, BLL13, BLG10, BRLS08, BRLS12, CC11, HS16b, KN$^+$12, LS11a, LLC$^+$10, LYS$^+$13, LWL$^+$10, Mat10, OAN15a, PML$^+$12, PdO$^+$16, PHK14, PD11, Pog10, PFVL14, RLD12, SPS$^+$12, Sch13, SWM10, SG10a, SG13, VLGK$^+$17, VVLG17, WX12, YOMT14, ZPP$^+$16, FL15]. Sets


**Similarities** [PM18]. Similarity [HS12, LMZ+11b, YDL+10, CDM10, CDB10, CDBM11, CQFC10, GWT+17, GK15b, HRK+10, HKRS11, HS11, RMPAM15, TZCK18, YZZ16, ZYvIZ14]. Similarity/dissimilarity [YDL+10]. SIMONA [SWB+12]. Simple [Ano15-59, CNK97, GM17, MPSA17, AB16b, BS10b, BD12, CWZB10, KRTB10, NS15, PHC13, PRIY+17, RHRC16, SEF+16, SS13c, dSAdSL13,
sites [AIGP15, Ano12a, DVVP14, DBK17, KDT+12, LZTV10, LHL+10, LL10b, LZX16, LG14, MA16, PHC13, PBG17, TYZ+16, Vor10, YZ15a, YHH+13, ZZL+12]. situ [JZL+17, LZY12b]. size [DMN15, BFH+13, BD12, CC12a, CF14, DJX+11b, FE14, GZ92, Hsu14, MTvG12, SL17, SB11, XYX17, Zha11]. Slater [Dil15, LRER13, MY17b, SFG+17]. Slater-function-based [SFG+17]. Slater-type [Dil15, MY17b], slices [AKN16], SLIM [SSBW14]. slit [Fom13]. slope [Zha12b]. SM [XMSZ16]. SM-TF [XMSZ16]. Small [XYW+14, ASS10, BTMS12, BLKP12, BS16b, CQFC10, DGL+13, ETLS17, GAMAC+14, GBFD12, KKPT11, KGHK12, KLJ+17, KB11b, KL13, LHKS12, LH14b, MSS+13, MBE16, MBRC16, MPBJ11, NH16, RLL+10, RS13, SG13, STS15, VT14, WF16, WTH+16, XML+15, XMSZ16, ZCGM11]. small-molecule [ETLS17, WF16]. smaller [MCK17b], smallest [PMT16]. SMD [ALK+15]. smeared [ENKK+17]. SMILES [TTB+10]. SMILES-based [TTB+10]. Smoluchowski [SG10a]. smooth [AG11, EFS16, JLCA17, ZSB+16]. smooth [LZ12]. SMPBS [XYX17]. Sn [MCK17b, PMG+16, RDT14, YW12, AS10, PKK17]. SnCl [dSDdAR10]. SmO [DHE+12]. Sodium [KLN16]. Soft [SJC11, Ben17, BG12]. Soft-core [SJC11, BG12]. Software [AIGP15, Aki16, APK14, AAC+16, BTA+13, BHB12, BCSCJ+13, BSZ+12, Ber17, BJP15, DMIN15, BFH+13, BBG+18, CBH14, CSEMB+16, CZAF17, CAT+13, DJD12, DVVP14, DDK14, DWC17, DSK17, ES13, EKW+13, FN12, FSC+14, GMSdG15, Gar12, GJMPAM+14, GLW13b, GS12, GCP+13, GCC14, GBW+14, GH16b, HLS+13, HRB+17, HDH12, HPT+16b, HPSK12, HHT+13b, HH16b, HG13, HYMZ16, HKR+14, HBJ+17, HL14, HC14, IK16, JHH+13, JJW+14, JLCA17, JP15, JCGM18, KS13a, KS15, KK17a, K15, KR14, KB16, KKR+13, KDR+18, KLJ+17, KJM+17, KDT+12, Kos16, KG13, KWL+16, KK17b, KWG15, KSD+12, KYG+15, KAG+12, KSW16, KPF+15, LPS12, LJ+12, LHSI12, Lhl15, LRvdS15, LRvE17, LDB+17, LLZA12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MDT16, MBR+15, MYT18, MSSF17, MB14, MB16, Nkj16, OV14, OPB+12, OZS+13]. Software [OC14, PSS14, PGL+15, DBDP16, PSG+17, PW12, PPM15, PHH+12, PVZ13, PG14, RLLH12, RNSF+16, Ras17, Rz216, RR14, Rda12, RSR+12, RCM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sic15, SJ17, SWB+12, SDMS13, TNY16, TSC+13, TTR+12, TTL+12, UU12, VMRS+17, VV+15b, VAR12, VB13b, WdV12, WY13, WPM+15, WF16, Web12b, WHK+12, WHJH13, WG14, WCJ+14, XML+15, XYX17, YW1+16, YZZ16, Yes12, Yes15, YHH+13, ZDKM12, ZLL+13, dVAG16, CCC+11, DFB14, MSvG12, MJG+15, SBV10, SGM+13, Yap11, ZCS+15, She12]. softwares [All11]. solar [ACS12, DGL+13, JYS+12, LTL+15a, SLC+17, TZ12, VAA14, YJN+11]. Solid [RSK+15, ASS10, ASK18, CL16, HLS12, HBI+17, KLN12, POG13]. Solid-state [RSK+15, ASS10, ASK18, CL16, HLS12, HBI+17, KLN12, POG13]. solids
solute

solutes

solubility

solute

solutes

solution

solutions

Solvation

solvation-free-energy

solvational

Solvatochromic

Solvatochromism

solve

Solvent

Solvent-driven

solvent-induced

solvent-dependent

solvent-dependent

Solvent-driven

solvent-induced

Solvvolysis

SOMA

Some

sometimes

spatial

sparsity

sparsity-weighted

Specific

specificity
Spectra
[PAK15, AMQ14, BG17, EBPK17b, FD13, FF11, GWF11, GGM12, GZZ12, HRH17, KASH14, Kow11, LBC12, LX11, MAK14, MCLD10, NHF10, PMC17, PDMT10, DCOD13, PDG16, RS17a, RJS17, SGDT10, SB15, SR11, TYN15, TZCK18, TG12b, Tsi14, WGL12, WWD14].
spectrometer [LBB15].
Spectroscopic
[SS13b, GK10, KDB13, Kop15b, NC13, NC14, TZCK18, Tsi14, ZLL10].
spectroscopy [HPSK12, LLBO12, NC12, WHK12].
spectroscopy-oriented [HPSK12].
speed [TO10, VM11, YD17].
speed-up [YD17].
speeding [AO10].
Sphalerite
[SBC11].
sphere [KT12, MH10, TH13].
spheres [HS16b].
spherical [Ano15-58, BH14, YOPB16].
spherically [Vyb15, Vyb16].
spheroidal [ZWY10b].
spider [Che17].
SPILLO [DVVP14].
Spin
[DSM11, JKS16, KM13, AB10, AMQ14, CSEMB16, CSS17, CSKH16, CAP17, FAA15, FD16, GP11a, KSK11, LXFC17, MG11, MCP18, PS17, RRK16, SFM14, SSB16, SH18, VFRAR16, YB11, ZLHH14].
Spin-component-scaled [KM13].
spin-coupled [SH18].
Spin-driven [DSM11].
spin-flip [ZLHH14].
Spin-orbit [JKS16, AMQ14, FAA15, FD16, GP11a, MG11, MCP18, PS17].
spin-polarized [SFM14].
SPINE [FZY12].
Spinar [CC12b, Bar14].
spins [ZR10].
Splitting [Rob13, EHSPT16, OT12].
SPME [NLP16].
SPOT [YZZ16].
SPOT-Ligand [YZZ16].
Spread [BEEL14].
Squaraines
[AMQ14].
square [HD14, IS14].
squared [JS13].
squares [BCCO10].
SR [ARAG17, WMW11].
SR-ZORA [ARAG17].
SrO [BL12].
SSC [LG11].
SSThread [Mau14].
ST [JJW14].
ST-analyzer [JJW14].
STAAR [JHH13].
stabilities [BLDK13, TFQ11].
Stability
[CSM16, EK15, GWT17, LiSRR16, OME16, PP10, BPPS17, CSS17, CFC15, CM16, CB11d, DLT17, DLW12, GPK16, Ham11, HLB15, LHKS12, MC10, MS15, PMG16, PAT10, Rab12, SY16a, TN12, XFTW15, ZRCC11, ZWMW10, ZWW10].
Stabilization [KSR17, BSDP16, DBK17].
stabilize [KG11].
stabilized [KASH14].
stacked [ANH11, HvM12, LDH14].
stacking [HvM12, YZZ17].
stages [CBP15].
Standard
[DH17, BCJC14, MKO13, PNI13, REL14, SRR16, VG13, WHK12].
standing [TS1].
staple [SV15].
State
[CCM16, GS16, Alg17, AR10, ASS10, BS15, BBI11, CSAOM17, CH10, CV12, ESM12, FD14, GS15, GCCM15, GPE13, HLS12, HNWFO7, HNWFO12, HHH16a, HHI17, HBI17, HZSS17, HBR17, JZ17, KLN12, Kop15a, Kop15b, KKL13, KCL14, LL15, LLBO12, LZL10, LYC13, LWGZ15, LN15, LGL11, LgV13b, LLFH16, LXFC17, MTM14, MPSG11, MCC11, MC12, MCLD10, NYM17, NMLD13, OBW12, OZLSBH12, POB13, PGW17, PH10b, QZ10c, RAGL11, RIJ11, RCM13a, RML15, RR14, RSK15,
SRF$^{+17}$, SSSM$^{15}$, SGWA$^{17}$, VZ$^{14}$, VL$^{17b}$, WHL$^{+10}$, WHX$^{+10}$, YWZ$^{14}$, YD$^{17}$, YYT$^{12}$, YL$^{13}$, Zim$^{15}$]. state-selected [KCL$^{+14}$]. State-specific [CCM$^{15}$, GCCM$^{15}$, LGL$^{11}$, LXFC$^{17}$, MCC$^{11}$, MC$^{12}$]. states [AST$^{+16}$, ANH$^{+11}$, BSL$^{+16}$, DHOG$^{13}$, EFS$^{16}$, EK$^{17}$, EP$^{15}$, FAA$^{15}$, FD$^{16}$, GO$^{13}$, GA$^{12}$, GTK$^{10}$, HDHL$^{15a}$, HDHL$^{15b}$, HDHL$^{15c}$, JCGVPHT$^{17}$, KB$^{14b}$, LLBO$^{12}$, LIW$^{12}$, LWW$^{12}$, LX$^{11}$, LS$^{11b}$, LYSS$^{11}$, MS$^{10}$, MN$^{15}$, MH$^{11}$, PBDW$^{11}$, RHRCH$^{16}$, SRF$^{+17}$, SOYC$^{12}$, ˇSB$^{13}$, ˇSB$^{15}$, SZZS$^{16}$, TN$^{10}$, Tia$^{12}$, TSN$^{17}$, VVV$^{+15a}$, XWSW$^{13}$, YZGS$^{14b}$, YK$^{13}$, YLZ$^{+10}$, YB$^{11}$, ZXS$^{+10}$, ZBB$^{16}$, dLC$^{17}$]. Static [KBC$^{12}$, BS$^{10a}$, KZK$^{+12}$, Lu$^{11}$, PC$^{14}$, PNW$^{+16}$, PM$^{13}$, WYT$^{17}$]. Statics [Pon$^{10}$]. stationary [BHR$^{15}$, Can$^{10}$, Can$^{11}$, LHMM$^{11}$]. stationary-point [BHR$^{15}$]. stationary-wave [Can$^{10}$, Can$^{11}$, LHMM$^{11}$]. Statistical [JHH$^{+13}$, PZA$^{15}$, PTB$^{+15}$, FL$^{15}$, GZ$^{14}$, HYMZ$^{16}$, ICS$^{+12}$, ICS$^{+13}$, Kan$^{15}$, KMLS$^{10}$, PTK$^{11}$, RB$^{13a}$]. statistically [GR$^{10a}$, GR$^{11}$]. statistics [QZ$^{10c}$]. steepest [MS$^{16}$]. steepest-descent [MS$^{16}$]. steered [FBEM$^{11}$, KERY$^{+16}$, MJC$^{14}$, NFG$^{+13}$, SJ$^{17}$]. step [AYYO$^{17}$, DS$^{12b}$, DGC$^{14}$, GRCL$^{12}$, JWO$^{15}$, JS$^{17b}$, KvdV$^{14}$, LLvG$^{10}$, LGL$^{11}$, LVG$^{13b}$, LL$^{10c}$, RLDJ$^{17}$, RS$^{12}$, SJC$^{11}$, TCP$^{14}$]. steps [REH$^{13}$, Zim$^{13}$]. Stepwise [DLP$^{11}$, GRCL$^{12}$, ZL$^{11}$]. stereodynamics [Chu$^{10}$, LWD$^{13}$]. stereoelectronic [AS$^{11}$]. Stereoselection [BJSI$^{12}$]. Steric [RMGR$^{11}$, MJLV$^{14b}$, MP$^{17a}$, YNH$^{+17}$]. sterically [MH$^{17}$]. Stern [MBA$^{11}$]. steroelectronic [HLBLC$^{15}$]. Stevens [BCJC$^{+14}$]. sticks [CVT$^{+11}$]. stilbene [BW$^{11b}$]. Stochastic [AFPI$^{13}$, CGP$^{12}$, AC$^{12}$, KV$^{12}$, KV$^{13}$, MS$^{16}$, MCP$^{18}$, NC$^{13}$, PH$^{17}$, RSL$^{13}$, SW$^{+12}$, VBD$^{11}$]. STOCK [BJP$^{15}$]. stoichiometric [VI$^{17}$]. stoichiometry [FSD$^{+18}$]. Stone [DWZ$^{+17}$, YZN$^{13}$]. stool [FPB$^{12}$, FB$^{14b}$, ZCK$^{+16}$]. storage [BEM$^{14}$, BEPM$^{14}$, DLT$^{17}$, WKLC$^{12}$]. Story [Sce$^{07}$, Sch$^{10}$]. Strain [DM$^{15}$, FB$^{12}$, FC$^{16}$, FLM$^{11}$, JWO$^{15}$, PBE$^{16}$, She$^{12}$, SHL$^{+13}$, VIT$^{+15}$]. strand [XYL$^{12}$]. strategies [AFBR$^{17}$, BSDP$^{16}$, cCVG$^{+14}$, DSX$^{+11}$, LTT$^{16}$, Rao$^{11}$, SOCJ$^{13}$]. strategy [CLX$^{+10}$, CZNA$^{11}$, HJK$^{13}$, KTNN$^{10}$, LLL$^{+10}$, PHC$^{13}$, PH$^{17}$, RVVK$^{13}$, TKNN$^{10}$, WO$^{15}$, XHHL$^{16}$, YDGZ$^{15}$]. strength [Fra$^{15}$, Fra$^{16}$, KSC$^{16}$, LGKS$^{17}$, MPSG$^{11}$, YJ$^{17}$, YHW$^{17}$]. strengthening [MS$^{11}$, LYSS$^{11}$]. strengths [CKL$^{+11}$, MLC$^{13}$]. streptavidin [MLZZ$^{12}$, ZJZM$^{13}$]. streptavidin-biotin [MLZZ$^{12}$]. streptocyanines [WYT$^{17}$]. stress [GMBX$^{+16}$, HXM$^{+16}$, JMX$^{+11}$, NIIT$^{15}$, NFI$^{+16}$, XFX$^{+16}$]. stretch [CK$^{10}$, RS$^{17b}$]. stretching [KLS$^{10}$, KMLS$^{10}$]. string [BMFG$^{16}$, JZ$^{17}$, Zim$^{15}$]. stringent [DPOS$^{16}$]. strong [Kan$^{15}$, MLZZ$^{12}$, SDF$^{12}$, VVY$^{17}$, Vik$^{11}$, ZSL$^{17}$]. stronger [KSC$^{16}$]. Structural [GLF$^{16}$, GBL$^{+11}$, GTT$^{10}$, GAMAC$^{+14}$, GWX$^{+12}$, HS$^{17a}$, II$^{10}$, KZK$^{+12}$, KSD$^{+12}$, LBTV$^{11}$, NC$^{14}$, TS$^{11}$, ZWW$^{10}$, AIGP$^{15}$, AD$^{10}$]
AKK+16, ALH+10, BBOB16, BPC13, CPV+12, CDS16, CYI+10, DWL11, DH11, GWT+17, HS17b, HVS16, KKPT11, KG11, KNE11a, KDT+12, LK13, LL13a, MCF10, PHC13, PGY15, PNG10, RR11, RKB+14, RSL16, SFA17, SS13c, WC11, XMSZ16, YVEI+17, ZYvIZ14, ZLW10, VPR10. structurally [TZCK18].

Structure
[BJP15, CGBK13, DXL+10, GPK+16, GWJJ12, GBGR16, HLB15, LAHS16, MHRR11, NC12, NC13, PMG+16, Rab12, SGH+16, VDVR14, WZK+13, AFIP13, AR15, AJR16, AC12, BPPS17, BFH+13, BddS13, CPRS18, CD13, CM13b, Clo15, DKE+17, DKT13, DDP16, DVVP14, DLW12, EH13, EKW+13, EFOD13, FZY+12, FSC+14, GLB16, GMSdG15, GRARO+14, GP12, GK10, GRD+10, GPdC+16, HASR+12, HNHR13, HS14a, HRB+17, HH15, HYMZ16, HZ13, HLWD15, Hua16, Ibr17, KYS+17, KSM17, K10, KS12, KKL+13, KLS10, KMLS10, LFB14, LKL10, LJJ+11, LMI+14, LYL16, LPE+10, LGL11, LHG11, LWWG12, LLFH16, Mat10, MDT10, Mau14, MAPB10, MV17, NGAS17, OCL11, OL13, OLA15, PSS14, PML+12, PN13, RLG14, RCM+13b, RR11, SHMO11, SB10, SM11, SLF+12, SLIB12, SRS14, SYN+12, SKGB13, TN12, TT+11, TGI2b, UNT16, VVF12].

structure [VHR16, VVBL17, VÅA14, VBMA13, VC110, VI17, VLGK+17, WO15, WRM+12, WSGN11, YW12, YZZ16, ZRC11, ZHHX11, OFS12, SA10].

structure-activity [DXL+10]. Structure-based [CGBK13, DXL+10, DVVP14, GLB16, VVF12].

Studies
[ISH10, KRTB10, OLY17, RHPWS13, RI10, TS15b]. Studies [JW12, AALCM11, BLS10, BRGN12, BLG10, DMN15, BIL10, DXX+10, GZMZ16, GEP+14, JLS+10, KG15, KP11, LXFC17, LCWW10, LJJ+11, LWD13, RCM+13b, SB10, SFA17, SLWH09, TDP+12, VSD10, WAC10, YKK+10, YPC+10, YDL+10, YXZZ17, ZZL+10, ZZL+10a, ZYG+15, ZXI11].

Study [JLH+14, VL17b, AAPP17, AS11, AS15a, AMAA+11, ASMS10, ANI+11, APA+14, APY+16, ALH+10, BEM14, BE14, BHB+17, BEEL14, BJS12, BLG11, BRLS08, BRLS12, BL12, BEL+11, CCLP14, CCLD14, CHWH11, CB17, CCJ+11, CKL+11, CXW14, CB716, CL16, CSX17, cCVG+14, ChA10, CG12, CB11c, CPL11, CB11d, DASA15, DR11, DL11, DLSD13, DSX+11, EOA+11, EV14, FCL+10, FF11, FCD10, FBEM11, FL15, FPB12, FB14b, GA14, GG10, GYX+10, GVP+10, GD10, GTK10, GWZ15, GNCA10, GGM+12, GKR13, GWPJ11, HZ11, HDB15, HD16, HRL11, HBR17, HVS16, Ibr11, IIF+10, INT+18, IN13, IHY15, II10, JA10, JS17a,
JCG+10, JAH+17, JJAB16, JW16, JYS+12, KD10, KKPT11, KOP+14, KC13b, KB13, KT12, KG11, KNK+12, KS13b, KP10, LC10, LY10, uLHY11, LP11a, LL13a, LL+10, LDJ+10]. study
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, Sc e07, Sch10, AAC+16, Fom11, JMS13, MGS+16]. **tables** [BDdS13, LZ12]. **TabBoo** [HTS15]. **tabu** [GBSE11]. **tabulated** [LL10a]. **tail** [MBC13]. **tailoring** [RKGN10]. **tails** [GSD10]. **Taming** [CCM15]. **Tamm** [HH17]. **tar** [HCD+10]. **tar-MD** [HCD+10]. **Target** [FMG12]. **TargetATPsite** [YHH+13]. **targets** [AFBR17, BK13, MPBJ11]. **Task** [CSSB11, HPSK12, KG13]. **task-oriented** [KG13]. **Task-parallel** [CSSB11]. **TATA** [YZWC11]. **Taurine** [YW13]. **tautomer** [WHJH13]. **tautomerism** [BJW13, LGOM+15]. **tautomerization** [BH13, BZH14]. **tautomers** [BZH14, dALdS+15]. **Tb** [SRL+15]. **TD** [CCB15, CH10, EFAC13, HRJ+15, JRSHP14, KKL+13, KP10, LZZ+10, LZHH11, LSH+11, LYSS11, RDF+11, SRF+17]. **TD-DFT** [CCB15, CH10, EFAC13, HRJ+15, JRSHP14, KKL+13, KP10, LZZ+10, LZHH11, LSH+11, LYSS11, RDF+11, SRF+17]. **TD-DFT-** [LSH+11]. **TD-HF-based** [LSH+11]. **TDDFT** [SFCCK+15, CMF+17, LRBB12, QCR12, SFCCK+14]. **Te** [HCD+10]. **technique** [AMGB10, BG17, LZL+13, SMM17, TSR+16]. **techniques** [BCP+10, BCG10, GVP+10, MCP18, 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, LL11, MK17, OGL10, TLdG+12, TM16, VED10, WMW11, YW12, OCW+15]. **Temperature-shuffled** [HS17b]. **temperature/Hamiltonian** [KCK+17]. **temperatures** [NMLD13, RHNN10]. **tempering** [LAW+16, MO15, MO17, NPTS16, TKT11]. **Template** [Man14, GLF16, KCK+17, ME10, YHH+13]. **Template-free** [Man14, YHH+13]. **template-restrained** [KCK+17]. **tension** [NFPD13]. **tensor** [Elk16, EWK+13, GMBX+16, HXM+16, JMX+16, KCK+17a, NFPD13, NIT+15, NFI+16, TKC+11, XFX+16]. **tensors** [EPD+11, PHK14]. **terahertz** [KB16]. **term** [DSF17, JBSQG11]. **terminal** [IMK+16, YXZZ17]. **terminally** [KLS10, KMLS10]. **terminally-blocked** [KLS10, KMLS10]. **terms** [BAS14, CZY11, CWZB10, RRH12]. **ternary** [RDT14]. **tertiary** [OPR16, SM11]. **tessellation** [MOS12]. **Test** [PHC13, BS10b, DPOS16]. **tested** [HMM10]. **Testing** [Gil11, II18, MPSA17, RLD12, JGS+17]. **tests** [Ano15-59, CNK97, ENKK+17]. **tethered** [CZNA11]. **tether** [WDG12]. **tetraamines** [SB10]. **tetracarboxylates** [CRC13]. **tetracoordinate** [XhD15, ZYW+16, ZLY+16]. **tetraene** [ABDG12]. **tetramer** [Ish10]. **tetramers** [LYL16, SZS16]. **Tetraoxide** [JW12, SLHWO9]. **tetraprotonated** [ZYW+10b]. **tetraradical** [Cas14, YSSB12]. **tetrasaccharide** [NPG17]. **tetrafluorovalene** [MC10]. **Tetrazine** [JW12, MCAG+16, SLHWO9]. **Tetrazine** [JW12, SLHWO9]. **Tetrazino-Tetrazine-Tetraoxide** [JW12, SLHWO9]. **tetrel** [YKH15].
tetroxide [MCAG+16], text [HKRS11, HS11], text-based [HKRS11, HS11], TF [XMSZ16], Th [MCK17a], their [ARRC15, Ano11, BSG18, CC12a, CBTZ16, CFC15, CB11a, DLT17, DSN+11, GPM17, HJ13, JMLL13, JHMB+09, JHMB+11, KG15, KENE11a, KRSCI12, NYH+17, SBR13, TN12, Tak11, TY10, TS11, VVJ15, VVY17, VVBL17, XDL+10, ZWY+10a, them [WCWV15], theorem [CDB10, KSH13, YB16, ZM11], theoretic [CRZ+18, MCC12, ZLW10]. Theoretical [AvKSP16, AMAA+11, BHB+17, BSDP16, CWT+12, DBM+17, DGL+13, FF11, GYX+10, GLZ17, GLM+17, HDHI15c, JW12, KCB+12, KS13b, LCL+10, LW12, LZW12, LWXC16, LXCFC17, LJG+11, MLQ+12, MSV16, NFI+16, OSS10, OAN15b, PKK17, PM13, PE11, RS17b, SB10, SKY+11, STS+10, SZSZ16, SLC+17, SGHL13, TPL+10, WMW11, WHDL11, WCL+11, WS12, YJN+11, YPC+10, YHC+11, YCGA10, YYT12, YDZG15, ZZL+10b, ZZL+10a, ZYLL12, ZLLL12, ZS1+14, ZYG+15, ZBMZH15, dSDLB17, BLS10, BE16, CZ12, CKL+11, CBTZ16, EV14, GG10, HDB15, HGH114, LW122, LLD17, LZW+11, MPSG11, NHH+10, NJX+10, PH12, PSE14, Pog10, PH10b, RZG+13, RVCF13, RVP+11, SSP+13, SJD11, SLHW09, SKTT11, SGH+16, Tak11, TL16, WSH10, WZQW10, YK13, YZWC11, YZN13, YB11, Zha12b, dSA1L3, HDHI15a, KZK+12, TDP+12, theories [OM12, WCWV15]. Theory [IU1+11, SZX13a, ZX13b, WM12, AMK11, ALK+15, AR10, ARAG17, ABGD12, AG12, ASS10, BY11, BLBG+13, BZB+13, BG13, CHG+16, CRZ+18, CSSdOM17, CWHH11, CK17, CCM15, CF14, CC11, DCHL12, FRSA14, FD16, GH17, GZL+12, GCCM15, GI10, GNGC10, GND12, GEG11, GP12, Han11, HPT17, Hii13, HNN+17, HRJ+14, HRJ+15, HG10, ISN13, IK13, IM17, JRSPH14, JLH+14, JW16, JYS+12, KHW17, KLN12, KM13, LCW12, LBGS16, LCL+10, LLH17, LPMT17, MCC11, MAK+14, MWJ+11, ME10, NMLD13, NO16, Niz13, ORZ11, OZLSBH12, PAK17, PML+12, PPH+14, Pie14, Py13, QZ10b, QZ10c, QB16, RAGL11, RJPB12, RCM+13a, RML+15, RB12, RSLML12, RHPWS13, Ruei11, SM14a, SFG+17, SCW11, SSSM15, SHF11, SEF+16, SE14, SH14, ST13, SHL+13, SMW09, SB14, SMM+18, SKTT16, SZZS16, STS15, TLdG+12, theory [TAG16, VDL+13, VVPI12, VV14, VL17a, VAMS14, WHL+10, WDLG12, WHX+11, WO15, WL14, WGN+16, XTY+14, XYW+14, YJ11, YLZ+10, YS13, YK15, ZXS+10, ZS1L12, ZLZ14, ZDX11, ZYG+14, ZWY+10b, ZWY+10a, ZLH+14, dSDS12a, dSDS12b, vLBFR12]. theory/configuration [HPT17], theory/time [JYS+12], therapeutic [AFBR17], therapy [ZZ12], there [MLGB16], Thermal [LL10c, ASL+11, BIL10, NGAS17, LZLSBH12], thermally [IIHY15], thermocalc [HDH12], Thermochemical [TFQ+11, KSM16, TN12, WDW12], thermochernistry [HDH12, Sán17, SB14, TCGNT18], Thermodynamic [EOO+16, PAT+10, BE12, BPE16, BB11b, BB11c, CBH14, CC18a, EBPK17b, HDL+17, Hug12, MMB+17, PGY15, PBE16, RNSF+16, RRF11,


Topological
[Jan16, AR15, PRYI+17, SB11, TSZQ12, VAR12, VBMA13, Wei12b, vSGP10].
topologies [Gar12, TSNC+17]. topology [AD10, ASS+17, Dil15, FED17, GMSdG15, KP11, MSSP17, yOaCG10, Rod13, dCDP15, BLG10].
topomerization [GG10].
toroidal [AD10, ASS+17, Dil15, FED17, GMSdG15, KP11, MSSP17, yOaCG10, Rod13, dCDP15, BLG10].
torque [Elk16].
torquoselectivity [GMBX+16].
torsion [SS13b].
torque [Elk16].
torsional [DPSL16, FZY+12, HP10b, HXM+16, JMX+16, YZ16].
torsional [BAS14, PRRT+10].
torture [RHT+11, TTL+12, TQ1/PC [VL17b].
torture [RHT+11, TTL+12, TQ1/PC [VL17b].
torus [WRG+17].
total [BEEL14, IKN13, MA16, SM16a, WX12].
toxicity [TTB+11, TTL+12, TQ1 [VL17b].
toxicity [TTB+11, TTL+12, TQ1 [VL17b].
track [ENKK+17, RHT+15].
track [ENKK+17, RHT+15].
tracking [BHR15].
tracking [BHR15].
tractability [KFY+13].
tractability [KFY+13].
training [DBDP16].
training [DBDP16].
trajectories [AST+16, HRID16, JZL+17, KG13, LZS+17, PSP15, RN17, SFR+11, ZSS+13, dSVdM+16].
trajectories [IUK+11, JJW+14, LWD13, LAS+14, MKS+12, PVZ13, SBD+17, Yu12a].
Trans [CSM16, MSBF16, BLS10].
Trans- [MSBF16].
Trans-2-Butene [CSM16].
transcription [XMSZ16].
transfer [Alg17, AK10, ANH+11, BHB12, CMF+17, CSAdOM17, CPL11, DWR17, DaDG15, EFAC13, ENKK+17, FC16, HSH15, HAP+12, HDHL15a, HDHL15b, HDHL15c, IYK11, JM11, JCGVPHT17, KGR+16, KDR+18, LZL+10, LLLM11, LWGZ15, LPLB16, MPSG11, MRB14, MSV16, PGCT+12, PAK17, PL14, PTB+15, Ras17, RCM+13a, RML+15, Ric16, REL17, RDLM14, SRF+17, SBD+17, SMP17a, SHB17, TM16, Tsi17, VKTRJ15, VMTL10, VL17b, WCT+11, WG14, XLY12, YKH+10, YLZ+10, YTT12, ZW17, dALdS+15].
Transferability [FP17a, ZRL+15, HOK17].
Transferability [FP17a, ZRL+15, HOK17].
transfers [YZGS14a].
transfers [YZGS14a].
transform [Ano15-58, BH14, Ish12, LL13a, SZTSM10, YWJ+16].
transform [Ano15-58, BH14, Ish12, LL13a, SZTSM10, YWJ+16].
Transformation [CCOH14, APY+16, DLW12, KZZ+16, REH13, RSK+15].
Transformation [CCOH14, APY+16, DLW12, KZZ+16, REH13, RSK+15].
transformations [HDL+14, SJC11].
transformations [HDL+14, SJC11].
Transiting [CM13a].
Transiting [CM13a].
Transition [OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GKI15a, GFGS18, GPE13, Hsu14, IYK11, JZ17, LYL16, LDZW17, LN15, LZW+11, LGKS17, LLL+12, MTM14, MS10, MN15, NMLD13, PHK14, RAGLL11, RIJ+11, SJZ+15, VVv+15a, YZGS14b, YWZ14, ZWW10, Zim15].
transition-metal [LDZW17].
transition-state [CSAdOM17, RAGLL11].
transition [LDZW17].
transition [LDZW17].
Transitions [AKK+16, BD11, DH11, HS17b, HB15, MCvdV13, PBDW11, SBT17].
Translationaly [MRO17].
Translationaly [MRO17].
translocation [MJC14].
translocation [MJC14].
transmembrane [DSF17, LMI+14, LAW+16, WXL+12].
transmembrane [DSF17, LMI+14, LAW+16, WXL+12].
transmission [LLJ12].
transmission [LLJ12].
transphosphorylation [WXY14].
transphosphorylation [WXY14].
Transport [DJX+11a, DMN15, CWHH11, CBTZ16, DMN14, DJX+11b, HLWD15, LHO17, LJ+12, NS17, PGY15, SLIB12, SY16b, TCX+13, ZYG+15].
Transport [DJX+11a, DMN15, CWHH11, CBTZ16, DMN14, DJX+11b, HLWD15, LHO17, LJ+12, NS17, PGY15, SLIB12, SY16b, TCX+13, ZYG+15].
transportation [LZY+12a].
transportation [LZY+12a].
trapped [DM15, VIT+15, WLV+10].
trapped [DM15, VIT+15, WLV+10].
Treating [JLCA17, SMP17a].
Treating [JLCA17, SMP17a].
Trends [CRP17, SMP17a].
Trends [CRP17, SMP17a].
tri [ZP13].
tri [ZP13].
tri-N-acetyl- [ZP13].
tri-N-acetyl- [ZP13].
tria
triadic [PPUBGD10]. triads [YKH+10].
triaminoguanidinium [ZYL+12]. triangles [She12]. triangular [TS11].
triangularly [LWZK13]. trianguenes [GSMM15]. triarylamine
[KGR+16]. triazine [WDLG12]. triazines [YPC+10]. triazol [ZZWT12].
triazole [NS10]. triazoles [GKR13, Ray13, RKG11]. trichlorostannate
[PKK1]. tricyclic [VSD10]. triel [Gra18, YKH15]. triene [ABDG12].
trifluoroethanol [JA10]. trifluoroethanol/water [JA10].
trifluoromethane [CLC11]. trifurcation [HOM+16]. triggered
[DAdGR15]. triggering [LLD17]. trigonal
[Ano11, Gav12, GRD+10, JHMB+09, JHMB+11]. trihalide [Gra18].
trihydrate [PM13]. trimer [THP+15, YCGA10]. Trimeric
[PMT16, RCM+13a, RML+15]. trimetallic [GLF16]. trimethylsilyl
[BIL10]. trinitrotoluene [SH14]. tripeptide [BH15, GMO16].
triphenylamine [MSV16]. triple [ACD+13a, ACD+13b, POB13].
tripeptide [POB13]. triplet [RS17a, THP+15]. triplets [EK15].
trNA [LBS10]. tropocollagen [PP10]. Trotter [VKAM12]. Trp [EJ13].
truncation [ACD+13a, ACD+13b, CS14, IMSR18, MC12]. trust [PLAG11].
trying [BRGN12]. trypanothione [VSD10]. tryptophan
[EOA+11, PS14, SHB17, VMTL10]. Tsallis [QZ10c]. TTTO
[JB12, SLHW9]. tuberculosis [MPNS13]. tubes [TS15b]. tubular
[uLhY11, ZLY+16]. tularensis [STM+15]. tumor [JAH+17]. tuned
[BK17b, HZSS17, SZS16]. tungsten [TS15a]. Tuning [Ano11, JHMB+09,
JHMB+11, BK17b, LWL+11, Mor15, RLG11, WYT17, LZ12]. tunnel [KL14].
tunneling [CSAdOM17, HS16a, LZW+11, OT12]. TURBOMOLE
[KK17b, RR14, STH+10, vV111]. tweezers [MBA14]. twelve [Pog10]. twist
[KTK17]. twisted [YLZ+10]. Two
[DS12b, Gra18, KKN11, KTO13, SC17, CCOH14, DPB+12, ECZWD17,
FRSA14, GAMAC+14, HLH+12, LPAS11, LRER13, NASH15, PS17, PW12,
SL14, SJC11, TCPC14, VT14, YAS13, YLL11, ZTH+15, SM17].
Two-Body [SC17]. two-center [LRER13]. two-component
[NASH15, PW12]. Two-dimensional [KTO13]. two-electron
[PS17, YLL11]. Two-level [KKN11]. two-phonon [DPB+12, ZTH+15].
two-scale [FRSA14]. Two-step [DS12b, SJC11, TCPC14]. type [BM12,
BE16, CYY+17, CRC13, CB11c, Dl15, HLWD15, JYC+16, LH14a, MY17a,
MY17b, MKH15, RKB+14, SZX13a, SZX13b, VED10, WvRSM14, ZX11].
type-II [CB11c]. types [SK+11, UT15]. typical [TZ12]. typing
[FP17b, YPKB12].
AKN16, HH10, HDMP+15, Ish10, KTO11, LMIP+14, OL13, ZZ14].

**unactivated** [YXZZ17], **unbiased** [ISO+13], **uncertainty** [Fer17, Han11].
**unconventional** [LDJ+10]. **uncoupled** [HH17]. **underlying** [RN17, SGPJS+17]. **Understanding** [DLZ15, Lun12, RCM+13a, TZ11, dCDP15, BH13, FCOGM12, KNE11a, LGVA14, LGKS17, VVJ15, ZK11].
**unexpected** [HYYZ13]. **Unexpectedly** [SDF12]. **Unfavorable** [MP17a, PRP15]. **Unified** [PPUBGD10, CVT+11, TNYN16].

**unique** [GS11, uLhY11]. **unit** [CKKK16, DZA11, DGL+13, EP10, Elk16, PMT16, SRL+15, WS13].
**unit-based** [WS13]. **Unitary** [SSSM15].

**unitary** [JGS+17, Jor17, ST11].
**units** [CCCLCGRO14, CYI+10, FCOGM12, GBL+11, HASR+12, HEMCZE+14, WSGN11, YWJ+16, YN15, ZKE+17].

**universal** [AH10, AJR16, Gar12, SYN+12].

**unknown** [GPdC+16, KYT+17, MFR10].

**unperturbed** [Gri13].

**unraveling** [HYYZ13]. **UNRES** [KMLS10, Sie15, SJ17]. **unrestricted** [BW11a].
**Unsaturated** [HPT16a, Tsi17].

**unsulfated** [SA10].

**ununoctium** [TH13].

**unusual** [KYCL11, LZJ+11].
**unzipping** [SM15, SM16b].

**Update** [CZAF17, MRO17, SPL+18, DPNM11]. **updated** [BCJC+14]. **Updates** [AIGP15, Ak16, APK14, AAC+16, BTA+13, BHB12, BCSJ+13, BSZ+12, Ber17, BJP15, DNN15, BFH+13, BBG+18, CBH14, CSEMM+16, CZAF17, CAT+13, DJD+12, DVVP14, DDK+14, DWC17, DSK+13, EB13, EWB+13, FN12, FSC+14, GMSdG15, Gar12, GJMPAM+14, GLW13b, GS12, GCP+13, GCC14, GBW+14, GH16b, HLS+13, HRB+17, HDH12, HPT+16b, HPSP12, HHT+13b, HH16b, HG13, HYMZ16, HK+14, HBJ+17, HL1+14, HC14, IGK16, JHH+13, JJW+14, JLA+17, JP15, JCMG18, KS13a, KS15, KI17a, Kan15, KB16, KDR+18, KLI+17, KJM+17, KDT+12, Kos16, KG13, KWL+16, KI17b, KG17G, KYG+15, KAG+12, KSW16, KFP+15, LPS12, LJR+12, LHSH12, Leh15, LRRvOM15, LRV+17, LDB+17, LLAZ+16, LB+15, LWZ+17, LC12, LAS+14, MHT+18, MDT+16, MBR+15, MYT+18, MSP17, MB14, MB16, NKJ16, OV14, OPB+12, OZS+13, OC14, PSS14, PGL+15].

**updates** [BBDP16, PSG+17, PW12, PPM15, PHH+12, PVZ13, PG14, RLLHL12, RNSF+16, Ras17, Rex16, RR14, RdA12, RSR+12, RCM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sie15, SJ17, SWB+12, SDMS13, TYN+16, TSC+13, TTR+12, TTL+12, UU12, VMRSH+17, VV+15b, VAR12, VB13b, WDN12, WDI3, WPM+15, WF16, Wei12b, WHK+12, WHJ+13, WG14, WCJ+14, XM+15, XXY17, YWJ+16, YZ16, Yes12, Yes15, YH+13, ZDKM12, ZL+13, dVAG16, KKR+13, SR18].

**updating** [UM13]. **upgrade** [ZSLL17]. **uptake** [WKC10a].

**uracil** [HvM12, LGOM+15, LJW11a]. **uracil/uracil** [HvM12]. **uranium** [OSS10].

**uranyl** [OSS10]. **URBOMOLE** [BBG+11]. **ureas** [FCL+10].

**ureido** [SSP+13]. **ureido-benzenesulfonamide** [SSP+13]. **uridines** [DPSL16].

**urokinase** [BM12]. **uroporphyrinogen** [BEL+11]. **uroporphyrinogen-III**
Use [DCOD13, GPM17, HCD+10, MPA12, MMZW14, NPTS16, NC14, NDD+10, RLDD12, WM17, Yes12, BCP+10].

[PGY15, Pie14, PLAG11, TH13]. Useful [SMGB11]. Usefulness [PSP15].


Using [BS15, Car14, DLL+10, HH10, HPSK12, LLvG10, LG14, MP11, QLQ11, SK17, TNG+10, WF16, AASP18, AG11, AGM+13, AC12, BW11b, BMR11, BDT11, BB11a, CVT+11, CAP17, CSSB11, DWL11, DBK17, DFF+15, DCHL12, DLZ15, EWK+13, FF11, FLM11, FL15, Gar12, GRS15, GFPSD17, GMO16, GZM11, GRL+10, LBB+15, LCH10, LCL+10, LMR14, LSG11, LTA+11, LBDP12, MS17, MZZ11, MRB14, MJC14, MN15, MY17a, MZ13, MKM+17, MCUI15, MVKS10, MKB+13, MFR+17, MIOM13, MJM10, M515, NLP+16, NASH15, NHH16, OCW+15, PGDO+16, PC11, PG15, Pia14, PJ13, RB13a].

using [RLDJ17, RDDS10, RJH11, RS13, RRK14, RIC16, REL17, REV+17, Ru11, RHG10, REN13, SMO11, SFM14, SDF+17, SVB10, SA13, SCW11, SFF+16, SHL+11, SKKS13, SY11, SRS14, SZZS16, STS15, TZY+16, Tak14, TKN10, TS17, TJB12, UTM11, VBAM12, VECT12, VI17, WKL12, WDYN12, WLC12, WZ17, WJX+10, WDHZ13, XTY+14, XYX17, XWW+11, YWJ+16, Yn16, YN15, YDX16, ZWLX11, ZL11, ZLT13, ZWS+10, ZP13, ZH12, ZHX11, dLC17, LHH+10]. Utility [YWVM12]. Utilizing [BVY+12].

UV [GGM+12, KASH14, RDF+11, RvdMB16]. UV-photoexcitation [RvdMB16]. UV/Vis [GGM+12].

V [WWKS16, LZL+15b, MG11, PBE16, WRM+12, WYGW12]. Valence [FF11]. Valence

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