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Title word cross-reference

\[ 1 \leq N \leq 6 \] [MPOC21]. \[ 2 \] [PSM+20, SLMA21]. \[ 3 \] [TT20]. \[ 4 \] [SS20]. \[ 5 \] [AS20, JMV21, SDK20, VTdlM20]. \[ 8 \] [Bal20b]. +
\[ APR21, CWZD20, LR20, WSV20 \]. − [WSV20]. \[ 2 \] [AKN+20]. \[ 2+ \]
\[ IK21, JRS20, SPSH20, ZRSST20 \]. \[ 3 \] [Mar21, TTDT20]. \[ 3 \] [MAR+20].
\[ 1 \] [Dor20], \[ 2 \] [AR20, DSC20, DBE20, DGSB+20, GGK20, MH20,
OKI+21, SWF+20, SWM+20b, TYZ20, TPZ+20, VTdlM20, WP20, WLZM20,
YYS20, YYZ+21, ZDBZ20]. \[ 20 \] [LR20]. \[ 0,±1,±2 \] [MIP+21]. \[ 2 \] [SLR+20].
\[ 3 \] [EK20b, EK20c, IK21, OE20, SLR+20, SL20, WLZM20, dCVARN20]. \[ 4 \]
\[ ZXZD20b, ZXZD20a \]. \[ 245 \] [HYA+20]. \[ 5 \] [OKI+21]. \[ 60 \] [DSC20]. \[ a \] [PWW20]. \[ N \]
\[ MPOC21, SLR+20, VTdlM20 \]. \[ 20 \] [TT20]. \[ 2 \] [ZDBZ20]. \[ 3 \] [JS21]. \[ 4 \]
\[ JS21 \]. \[ 5 \] [CSP20, SSS+20b]. \[ 6 \] [AV20, BPDG21, KgD+21]. \[ 7 \] [OE20, OE20],
\[ \cdots \] [BdLC21, TT+21]. \[ d \] [IK21]. \[ 8 \] [EK20a]. \[ f \] [SCZ+21]. \[ \lambda \] [Ngo21]. \[ \log P \]
\[ [DHD21]. \[ \mu \] [MVP+20]. \[ \n = 1 \] [TT20, VTdlM20]. \[ p \] [AR20]. \[ \pi \]

-dependent [Ngo21, JRS20]. -diaqua [MVP+20]. -diketones [AV20].

/CBS [CSWW20, Dor20, SK20]. /H [WSV20].


2 [CM20b, KGD+21, ONA+20, RLR+20, SLR+20]. 2-HOPO [SDK20].

4-triazole-3-thione [KGD+21]. 40 [MT20a].

6-lutidine [TYZ20]. 60th [IBL20].

7 [CM20b]. 7D [Bal20a]. 7D-Hypercube [Bal20a].

8-hydroxyquinolinato [AS20].

= [AS20, APR21, MH20, SL20, ZDBZ20].

AQUA-MER [ALGDock [Min20]. algebra [GJMPVR+20].

Algorithm [AlIS+21, WSL+20, FR21, JKK+21, MB21, SS20]. algorithms [GWN21].


Amorphous [XZZ+20]. analogues [SJZ+21]. Analyses [SLR+20, AK20, TS21]. Analysis [AKR21, AD20, KUNT20, MH20, BdLC21, CJKH21, CSP20, CB20, ETT21b, EK20c, EPT21, HL20, JMK+20, JRS20, MDO+20, MT20b, NTK21, NEG+20, RCC+20, RA20, YIO20, ZGZC20].


Combining [WSL+20, NML21].

Comment [MT21, NTK21, CPG21]. communications [AiIS+21].

Comparative [JMV21]. compared [WD20]. Comparison [CN21, SK20].

compatible [PLP+20], competition [SJZ+21]. Complete [HL20, SCKH21].

complex [ALA20, KLT21, OE20, SWF+20, TM20, YYS20, ZMH+21, ZZG+21].

complexation [SDK20]. Complexes [AD20, BGS+20, ASL+20, AS20, LKT21, MVP+20, PB20, SVDS21, SEZ20, SD21, YFS20, dBCdl20].

component [KL20]. components [AV20, NTK21]. composite [WD20].

Comparison [CN21, SK20]. compatible [PLP+20]. competition [SJZ+21]. Complete [HL20, SCKH21].

complex [ALA20, KLT21, OE20, SWF+20, TM20, YYS20, ZMH+21, ZZG+21].

complexation [SDK20]. Complexes [AD20, BGS+20, ASL+20, AS20, LKT21, MVP+20, PB20, SVDS21, SEZ20, SD21, YFS20, dBCdl20].

component [KL20]. components [AV20, NTK21]. composite [WD20].

Contact [CLS+20]. Contacts [MKSS20]. containing [CTBB20, NST+20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].

Conformations [TPZ+20, SS20, STR20, TTH+21a, WSV20, ZGZC20]. Conformers [ONC20]. conical [AV20].


[HRT+20, Min20]. flip [IYI+20]. Flow [BSL20]. fluid [CM20a]. fluids
[SSYB+20]. fluorescence [AS21]. fluorescent [ZRSST20]. Fluorine [OE20].
flux [MNZGO+20]. fly [OSHT20]. focal [BSF20]. focal-point [BSF20].
Fock [BBK20]. Fold [CLS+20]. folding [SSS+20b]. Following
[CG20, ETT21b]. Force [BAC20, LJ20, QB20, WSL+20, DHD21, FVSS20,
KYM20, MT21, MNZGO+20, ODL20, PLP+20, YFH+21]. forces
[KSP21, LCC+21]. Form [CWZD20]. Formation
[GOY20, HL20, MDO+20, SSS+20a]. formats [VAP+21]. forms [DSC20].
Fourier [YLZ+20]. Fractional [ASW20]. Fragment
[CLS+20, KUNT20, AKN+20, BBC+21a, UB20]. fragment-based [UB20].
Fragment-Free [CLS+20]. Fragmentation [AKN+20, SD21]. Framework
[GRN20, LPP20, CM20a, GUCCR20, HRTSS+20, WMZJ20]. frameworks
[WP20]. Free [BBC20, CLS+20, FMFG20, GBM20, MXM20, Min20,
NNT+20, SZLD20, CSP20, HB21, HBM+20, MN20, MB21, NML20, ÖLP+20,
SY21, TM20, TYZ20, YBS+20, YIO20]. Free-energy [GBM20, SY21].
friendly [SKS21]. fromage [RDS+20]. FSATOOL [ZGZC20]. Fukui
[GUCCR20]. fullerene [AK20]. fullerenes [WKCP21]. function
[AV20, KFTB20b, SWF+20, WMZJ20, YFH+21]. function-based [AV20].
Functional
[BBK20, CWZD20, SK20, YXGZ20, APS20, AS21, BWS20, CPG21, CTBB20,
DZL+20, FB20, HCS+20, IYI+20, MKW+20, HI20, MSS20, NEG+20, NN20,
OE20, OM+20, SDK20, dASRHBB21, SSYB+20, SZP+20, WKCP21, ZGZ+20].
Functionalized [LR20, YYZ+21]. functionals
[BOPJ+21a, GAP21, HCS+20, MN20, NG20, WS21]. Functions
[GVMB+20, GUCCR20, SM20, SCZ+21]. Fuzzy
[GVMB+20, GJMPV+20].

G [BWM20, CD20, WGKG20]. G-protein [WGKG20].
G-Protein-Coupled [BWM20]. Ga [AS20]. gas [APR21, WG20]. Gaussian
[GRN20, LB21]. Gaussians [ALA20]. Ge [SGT+20]. General
[Gao20, VCL20]. Generalized [GCL+20, HTFY21, VV20b, NG20, XCJ20].
Generalized-ensemble [HTFY21]. Generating [SHM+20, VAP+21].
Generation [AMF+20, DYGM21, Gao20, TIK21]. genetic [SS20].
Geometric [ETT21b, DHD21]. geometrical [GJMPV+20]. geometries
[NG20, WD20]. Geometry [LPP20, MMK+20]. GFP [RPD+20a]. giant
[WKCP21]. GIAO [MPOC21]. GIAO-NMR [MPOC21]. Glioblastoma
[CM20b]. Global [CPG21, MZ21, OKI+21, TTH+21a]. Glycans [KUNT20].
glycine [HB21, ONC20]. glycoprotein [ONA+20]. glycoprotein-enhanced
[ONA+20]. glycosaminoglycans [MZMK+21]. gold [LL21, NST+20].
grain [NG20, VV20b]. gradients [BSF20, VCL20]. grafted [GBM20].
Grained [MT20a, WSL+20, WZZ+20, GWN21, MT19]. grand [GGK20].
grand-canonical [GGK20]. graphene [BWS20, DZL+20, YC20, dCRM21].
grahene-supported [BWS20, DZL+20]. Graphical [SBG20]. Graphics
[GCL+20]. Graphs [SBG20, DHD21]. grasp [BPDG21]. Gremlin [CM20b].


identified [SSYB+20]. Identifying [PAS+20]. II [AB20b, AD20, SVDS21, SSS+20a, YYS20]. III [AS20, HRTSS+20]. ILE [MPOC21]. Image [ABZ20a, ANo20a, Ano20b, Ano20p, Ano20t, Ano20u, Ano20v, Ano20w, Ano20x, Ano20y, Ano20z, Ano20-27, Ano20-28, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20l, Ano20m, Ano20n, Ano20o, Ano20p, Ano20q, Ano20r, Ano20s, BBC+21b, BOPJ+21b, ETI21a, KFRB20a, RP+20b, SWM+20a, dRHB21, TTT+21b, VV20a]. imino [YFS20]. immersive [MSL+20]. Immunodeficiency [KUNT20]. impact [SPSH20]. Implementation [YLZ+20, CSGV+20, CPG21, FR21, OMC+20]. implications [KSP21]. Implicit [GCL+20, RP+20a]. Importance [HKSW20]. improbability [RLR+20]. Improved [BBK20, LJ20].
incorporating [Gie21]. incorrectly [GAP21].

increase [LKM20]. increases [HREvdK+20]. independent [LGC21].


Information


infrared [GPEK+20, PGP+21]. inhibitor [BAO20].

inhibitors [KGD+21, MPuS+20, PWX+20]. inhibits [HTFY21].


interacting [CSGVF+20, JGGPN21]. interaction [KUNT20, PT20, dCRM21, AA20, ASW20, BdLC21, CSWW20, HTFY21, PHS+20, WMZJ20].

Interactions

[BWM20, LJ20, WP20, BRNB21, BPDG21, CM20b, CTBB20, EPT21, HPG20, HTFY21, KGD+21, ODL20, OE20, YW20]. Interatomic [AA20, ZFRM20]. intercalation [HKSW20]. interesting [HPG20].

interface [SNN+21]. interfacial [CM20a]. intermediate [MMK+20].

Intermediates [SK20]. Intermolecular [KGD+21, OOY20, HTFY21].

Internal [WZZ+20, BLB20]. Interplay [HYA+20, ZRSST20].


intramolecular [AIV20, CRT+21, KSP21, RA20]. Intrinsic [AD20]. intrinsically [SY21]. Introducing [SKS21]. invariant [KSRB+21].


IOData [VAP+21]. Iodido [SVDS21]. Iodine [ASL+20, SCZ+21]. Logansen [TTT+21]. Ion [SLR+20, FVSS20, HPG20, JRS20, LA20, XAD20].

ion-induced [FVSS20]. Ion-Pair [SLR+20]. Ionic [VAL20, XAD20].


Isoelectronic [ZXD20a, ZXD20b]. isolated [JS21]. Isolation [BLP20].

kesterites [MZ21]. Key [VV20b], kinematic [HC21], kinetic [EG20, JMK+20, dCVARN20]. Kinetics [SK20, CD20, DWSX20]. Kohn [EK20a, HCS+20, MB21]. Koopmans [GX20].


n [ZDBZ20, DZL+20, MKSS20, PAS+20]. N-co-doped [DZL+20].

Rhodopsins \([\text{HREvdK}^+20]\), riboswitches \([\text{AAe}20]\), ribozyme \([\text{JRS}20]\), rich \([\text{JM}V21]\), right \([\text{SCZ}^+20]\), Rigid \([\text{Min}20]\), Ring \([\text{LJ}20]\), RISM \([\text{YIO}20]\), \(\text{Rn}\) \([\text{APR}21]\), \(\text{RNA}\) \([\text{AAe}20, \text{TM}20, \text{YFH}^+21]\), robust \([\text{NMFI}21]\), Role \([\text{MKSS}20, \text{MAP}^+20, \text{LKT}21]\), roles \([\text{VV}20]\), Roux \([\text{IBL}20]\), RS \([\text{VAL}20]\), RuBisCO \([\text{DGSB}^+20, \text{JMK}^+20]\), rule \([\text{TTT}^+21]\), ruthenium \([\text{YYS}20]\), route \([\text{VTdlM}20]\).

S \([\text{DBE}20, \text{Gic}21, \text{SLR}^+20, \text{PWW}20]\), SA \([\text{Sts}20]\), SA-2-CASSCF \([\text{Sts}20]\), salts \([\text{JM}V21]\), same \([\text{Sán}20]\), same-spin \([\text{Sán}20]\), Sampling \([\text{FMFG}20, \text{AKR}21, \text{KSRB}^+21, \text{LG}C21, \text{Ngo}21, \text{SSS}^+20a, \text{STR}20, \text{ZGZC}20]\), SARS \([\text{ONA}^+20, \text{SLMA}21]\), SARS-CoV-2 \([\text{ONA}^+20]\), scalar \([\text{RN}^+20]\), scale \([\text{BGS}^+20, \text{CJH}W21, \text{HR}EvdK^+20, \text{JKK}^+21, \text{RDS}^+20, \text{SY}21]\), scaled \([\text{Sán}20]\), sampling \([\text{AS}W20, \text{MZMK}^+21, \text{SE}20]\), scattering \([\text{D}H\text{D}21, \text{MH}20]\), Scheme \([\text{BSL}20, \text{GRN}20, \text{FCGP}20, \text{Gao}20, \text{MT}20b, \text{RH}21, \text{STR}20]\), schemes \([\text{DO}20, \text{HD}21]\), schiff \([\text{ZRSS}20]\), Science \([\text{PAF}^+20]\), scoring \([\text{AMF}^+20]\), scramblase \([\text{KCF}^+20]\), screened \([\text{YW}20]\), screening \([\text{AR}20, \text{CJH}W21]\), Secondary \([\text{AD}20, \text{AAe}20, \text{HC}21, \text{JRS}20, \text{KSRKS}21]\), sections \([\text{ALA}20, \text{dBCdL}20]\), selected \([\text{CN}21]\), selected-CI \([\text{CN}21]\), selective \([\text{HRTSS}^+20]\), selenium \([\text{ZGZ}^+20]\), selenium-containing \([\text{ZGZ}^+20]\), self \([\text{AS}W20, \text{CQSG}20, \text{MAP}^+20, \text{PRH}20, \text{SKK}20]\), self-assembly \([\text{MAP}^+20, \text{PRH}20]\), self-consistent \([\text{CQSG}20, \text{SKK}20]\), self-interaction \([\text{AS}W20]\), semi \([\text{PWX}^+20]\), semi-empirical \([\text{PWX}^+20]\), semiconducting \([\text{CBF}^+20]\), semiconductor \([\text{L}M\text{PT}21, \text{ZGZ}^+20]\), Semiempirical \([\text{GUCC}20, \text{Gic}21]\), Sensing \([\text{HRTSS}^+20]\), sensitivity \([\text{LG}M20]\), sensor \([\text{ZRSS}20]\), Separated \([\text{BBK}20]\), separation \([\text{WG}20, \text{YYZ}^+21]\), sequence \([\text{KSRKS}21]\), sequence-based \([\text{KSRKS}21]\), sequential \([\text{GGK}20]\), series \([\text{PWX}^+20]\), server \([\text{LGD}^+20, \text{MPuS}^+20]\), Set \([\text{XZ}20, \text{YXGZ}20, \text{SCKH}21]\), sets \([\text{LB}21, \text{RNP}20]\), Sham \([\text{EK}20a, \text{HCS}^+20, \text{MB}21]\), Shavitt \([\text{SBC}20]\), shell \([\text{AME}^+21, \text{MB}21, \text{Sán}20]\), shift \([\text{TTDT}20, \text{UB}20]\), shock \([\text{BAO}^+20, \text{FVSS}20]\), short \([\text{HTFY}21]\), short-range \([\text{HTFY}21]\), side \([\text{OD}L20, \text{SSS}^+20b]\), side-chain \([\text{SSS}^+20b]\), Silicon \([\text{HZG}^+20, \text{GPEK}^+20, \text{PGP}^+21, \text{ZXD}20b, \text{ZXD}20a]\), similar \([\text{HGF}20]\), Simple \([\text{RH}21]\), Simplex \([\text{WSL}^+20]\), simulate \([\text{TTT}^+21]\), Simulating \([\text{LA}20, \text{AME}^+21]\), Simulation \([\text{HZG}^+20, \text{NNT}^+20, \text{PAF}^+20, \text{SL}20, \text{BBC}20, \text{CSP}20, \text{CBB}^+21, \text{HR}EvdK^+20, \text{HBM}^+20, \text{KCG}20, \text{ON}A^+20, \text{SNN}^+21, \text{SY}21]\), Simulations \([\text{SZLD}20, \text{Zac}20, \text{DO}20, \text{EK}20a, \text{GGK}20, \text{LL}21, \text{LKM}20, \text{LGC}21, \text{MPOC}21, \text{Ngo}21, \text{NN}20, \text{PDL}^+21, \text{QLC}^+20, \text{RGGD}21, \text{SKKK}20, \text{WGK}20, \text{WK}D^+21]\), single \([\text{AK}20, \text{CBF}^+20, \text{KSRKS}21]\), single-molecule \([\text{AK}20]\), single-walled \([\text{CBF}^+20]\), Singlet \([\text{HFP}20, \text{SCKH}21]\), singular \([\text{MT}20b]\), Site
[VDK⁺20, BBC20, DPSG20, KGD⁺21, PLP⁺20]. sites
[HGF20, LKM20, YIO20]. sixth [LB21]. size [HKSW20, JS21, XAD20].
size-modified [XAD20]. Sized [MFC20, ZDBZ20]. slab [VTdlM20]. Slater
[FV20]. slip [WKD⁺21]. slip-springs [WKD⁺21]. Small
[LPS20, JS21, KYM20, NST⁺20, TIK21, YIO20, ZDBZ20]. small-sized
[ZDBZ20]. Smoothed [GJMPB⁺20]. Software
[Zac20, AME⁺21, CJHW21, GJMPVR⁺20, SNN⁺21]. solar [SZP⁺20]. solid
[EG20, LB21]. solid-state [LB21]. Solute [GRN20]. solution
[MPOC21, RPD⁺20a]. solutions [KSRB⁺21, SSS⁺20a]. Solvation
[GRN20, MFC20, NML21, RPD⁺20a]. Solvent
[BBK20, FMFG20, GCL⁺20, SLR⁺20, Srs20, SPSH20, VCL20, XAD20].
solvent-accessible [VCL20]. solvents [RPD⁺20a]. solving [MB21]. Some
[QB20]. source [FR21]. sp [AKN⁺20]. space [BAO⁺20, HL20]. speciation
[LG⁺20]. species [XAD20]. specific [WRBT21]. Spectra
[CWZD20, EK20a, GPEK⁺20, PGP⁺21, SN⁺21, TMÖ⁺21]. Spectroscopy
[BLP20, FB20, MPOC21]. spectrum [AS21]. speed [GW21]. Spherical
[GJMPB⁺20]. SPIDER3 [KSRKS21]. SPIDER3-single [KSRKS21]. spike
[ONA⁺20]. Spin [IYI⁺20, SWF⁺20, SWM⁺20b, HYA⁺20, PHS⁺20, QLC⁺20,
S₂n20, VV20b, XC20]. spin-coupled [XC20]. Spin-flip [IYI⁺20].
Spin-inversion [SWF⁺20, SWM⁺20b]. spin-orbit [PHS⁺20]. spin-pair
[QLC⁺20]. splitting [OSHT20, YYS20]. splittings [SRB21]. SPOT
[CLS⁺20]. SPOT-Fold [CLS⁺20]. springs [WKD⁺21]. stabilities
[VCL20]. Stability
[STB⁺20, VAL20, APR21, BPDG21, MIP⁺21, PB20, VTdlM20].
stabilization [PFSC20]. Standalone [KYM20]. stannites [MZ21]. State
[BWM20, BSF20, AIV20, HD21, KL20, LB21, OSHT20, Srs20, WD20,
WMZ20, ZRSST20, dCVARN20]. State-of-the-art [BSF20]. states
[CG20, CPG21, FB21, Gie21, HYA⁺20, IK21, OMC⁺20, RDS⁺20]. Statistical
[DSGB⁺20]. stereographic [VCL20]. Stereoselectivity [WLZM20].
Steric [VDK⁺20]. stone [CTBB20]. stone-wales [CTBB20]. storage
[SSYB⁺20, WG20]. Strain [SLR⁺20]. strategy [HB21]. strength
[CVGN⁺20, MVP⁺20, NTK21]. Streptomycetes [CD20]. stretching
[GAP21]. strong [FCPG20]. strontium [KGG21]. Structural
[CM20b, PSM⁺20, SL20, ONA⁺20]. Structure
[CLS⁺20, MIP⁺21, XZ20, AAc20, AYO20, BLB20, DGB⁺20, GAG20, HC21,
HGF20, MZ21, VTdlM20, WS21]. Structures
[CWZD20, HZG⁺20, DYGM21, KSRKS21, TT20, YIO20, ZDBZ20]. studied
[LL21, SY21, WS21]. Studies [CWZD20, HKSW20, ZFRM20]. Study
[JFZ⁺20, APS20, BBC20, CS20, CTBB20, CRT⁺21, DZL⁺20, HTFY21,
JC20, JM21, KSRB⁺21, MNZGO⁺20, MAP⁺20, OE20, OSM20, PRH20,
RPD⁺20a, RDS⁺20, dASRHB21, SVDS21, SSS⁺20a, TMO⁺21, TFP⁺20,
VTdlM20, WG20, WRBT21, YYS20, ZDBZ20, ZMH⁺21]. styrene [ZZG⁺21].
substituent [LGM20]. Substituted [NRH⁺20, ASL⁺20, MNZGO⁺20].
Superposition [Wan21]. supported [BWS20, DZL+20]. supramolecular [GBM20]. Surface
[GCL+20, MH20, PAF+20, YXGZ20, FCPG20, OK1+21, SZP+20, VCL20].
symmetry-adapted [NTK21, OE20]. synergistic [PRH20]. System
[HL+20]. Systematic [KUNT20, STR20, TS21]. Systems
[LR20, JKK+21, UB20, WG20, YAO20].

T [CS20, CSWW20, Dor20, PRF20, Sts20]. Taba [dSBFdAJ20]. table
[GWN21]. TaH [WLZM20], tailoring [AV20]. tangential [CBF+20]. target
[SLMA21]. TD [MPOC21, WD20]. TD-DFT [MPOC21]. TDDFT
[NRH+20, Sts20]. Technique [WSL+20]. techniques [MZ21]. tempering
[LGC21]. tensor [GJMVR+20]. Terminal [FZ+20, MKSS20].
tetrahydrodibenzoazines [SS20]. tetrikis [MVP+20]. tetrapeptide
[MAP+20]. tetrahedral [SDK20]. Tf [TYZ20]. TGR5 [WKG20].
thiophylline [TM20]. theophylline-RNA [TM20]. theorem [GX20].

Theoretical
[JM+20, VTdlM20, HRTSS+20, MNZGO+20, NMFI21, OSM20, PRH20].
Theory
[IYI+20, SK20, YXGZ20, APS20, AS21, ASL+20, AA20, BWS20, CPG21,
CTBB20, DZL+20, FB20, FKT21, GX20, HCS+20, LGM20, MKW+20,
MH20, MSS20, NTK21, NEG+20, OE20, OMC+20, RGGD21, SDK20,
SFH+20, San20, dASRB21, SSYB+20, SZP+20, WKCP21, dCVARN20].
therapy [ASL+20]. there [dCRM21]. thermal [GGK20]. Thermochemical
[WKCP21, SSYB+20]. Thermodynamic [DBE20, SZLD20, KCGK20].
Thermodynamics [SK20]. Thioflavin [Sts20]. thioguanine [NST+20].
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