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Title word cross-reference

1 \leq N \leq 6 [MPOC21]. 2 [PSM+20]. 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]. ′ [PAS+20]. 1
[Dor20], 10 [LR20]. 2
[AR20, DSC20, DBE20, DGSB+20, GGK20, MH20, OKI+21, SWF+20,
SMW+20b, TYZ20, TPZ+20, VTdlM20, WP20, WLZM20, YYS20, ZDBZ20].
2 [LR20]. \cdot \cdot [MIP+21]. \cdot [SLR+20]. 3
[EK20b, EK20c, IK21, OE20, SLR+20, SL20, WLZM20, dCVARN20]. 4
[ZXD20b, ZXD20a]. 450 [HYA+20]. 5 [OKI+21]. 60 [DSC20]. a [PWW20]. N
[MPOC21, SLR+20, VTdlM20]. \cdot \cdot \cdot [TT20]. \cdot \cdot [ZDBZ20]. x [JS21]. \cdot
[JS21], \alpha [CSP20, SSS+20b], \beta [AV20, BPDG21, KGD+21], \cdot [OE20, OE20],
\cdot \cdot [TTT+21], d [IK21], \Delta [EK20a]. f [SCZ+21], \lambda [Ngo21], \mu [MVP+20].
\( n = 1 \) [TT20, VTdIM20]. \( p \) [AR20]. \( \pi \) [AV20, CBF\(^+\)20, LJ20, ODL20]. \( \sigma \) [AV20].


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

1 [CM20b, KUNT20, PWX\(^+\)20, Sán20]. 1-11 [ZDBZ20]. 10.1002/jcc.25747 [MT20a].

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

3D [YIO20]. 3D-RISM [YIO20].

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].

Alder IMNZGO + 20, SSYB + 20. AlgDock [Min20].

Alden [GJMPVR + 20]. Algorithm [WSL + 20, JKK + 21, MB21, SS20].

Alkal [JMV21, ODL20, OSM20]. Alkylation [MAP + 20]. Alkene [WLZM20].

Alkynes [JFZ + 20, TY20]. all-atom [LKM20, WGKG20]. All-electron [RNP20]. all-purpose [Mar21]. Allosteric [BSL20]. along [CG20].

An [AMgF + 20]. amine [HPG20]. amino [HREvdK + 20, ODL20]. aminotetrazole [JMV21]. aminotransferase [BBC20]. Ammonia [MFC20, SPSH20].

Ammonium [ODL20]. AMOEBA [PLP + 20]. among [DWSX20].

Amorphous [XZZ + 20]. Analyses [SLR + 20, AK20, TS21]. Analysis [AKR21, AD20, KUNT20, MH20, CJHW21, CSP20, CB20, EK20c, EPT21, HL20, JMK + 20, JRS20, MTO + 20, MT20b, NTK21, NEG + 20, RCC + 20, RA20, YIO20, ZGZC20].


Basis [YXGZ20, CM20b, RNP20, SCKH21, SM20]. bath [CQSG20].
batteries [SGT+20]. Be [ZDB20]. behavior [AK20]. Bel
[ZXD20b, ZXD20a]. benchmark [CGP21, CS20, DGSB+20, OMC+20].
Benchmarking [ZXZ20]. Benoit [IBL20]. bent [WG20]. benzene
[NMF21, XCI20]. beryllium [ZDB20]. beryllium-doped [ZDBZ20].
between [CS20, CTBB20, HYA+20, Min20, NTK21, SSS+20b]. bias
[KSRB+21]. biased [RGGD21]. biased/accelerated [RGGD21].
bifunctional [HBM+20]. bile [WGKG20]. Binding
[GOY20, NXM20, Min20, NNT+20, SZLD20, dSBFdAJ20, BRNB21, CSP20, HGF20, IYI+20, NTK21, Ngo21, NST+20, NN20, ÖLP+20, PWX+20, SWF+20, SWM+20b, SSO+20, WKCP21, YIO20]. bioactivity [MPuS+20].
Biological [AWID+20, JK20, SS20]. biology [IBL20]. Biomolecules
[WZZ+20, ZGZC20]. biophysical [SKS21]. biosystems [GUCCR20].
birthday [IBL20], bis [YFS20]. Block [RA20, AR20], blocks [RA20]. Blue
[HBM+20]. BMP [CM20b]. BMP-2 [CM20b]. BMP-7 [CM20b]. BODIPY
[FB21]. BODIPY/Aza [FB21]. BODIPY/Aza-BODIPY [FB21]. body
[PDL+21]. bonding [AV20, AA20, BGS+20, CCVGN+20, EK20c, JC20, MVP+20, MIP+21, NEG+20, dBcL20]. bonds
[CB20, NTK21, SD21, WG20]. borane [ZZG+21]. Born [GCL+20]. both
[KCF+20, PRH20]. boundary [YAO20]. bpy [IK21]. Br [GGK20].
brakeage [FVSS20]. Breakdown [AD20]. Breaking [LR20]. breathing
[CBF+20]. brevicompactum [HYA+20]. Bridging [HZG+20]. Brownian

C [LR20, OKI+21, ZFRM20, DZL+20, DSC20, MPuS+20]. cage
[DSC20, GGK20]. CAI [XZD20a]. CAI [XZD20b]. calculate [SS20].
Calculation [Sän20, CSWW20, ÖLP+20, PRF20, VCL20, YBS+20].
Calculations [DBE20, MXM20, Min20, DGSB+20, EK20b, EPT21, FV20, FB20, GBM20, HRTSS+20, KL20, Mar21, PFSC20, QLC+20, SRB21, SWF+20, SWM+20b, SSS+20, TM20, TT20]. Calibration [DP20].
camptothecin [PRH20]. cancer [SVS21]. canonical [GGK20, KSRS+21].
Carbenes [PAS+20]. Carbocyclic [PAS+20]. Carbon [ZXD20a, APS20, AS21, AKN+20, CBF+20, CTBB20, GPEK+20, ZSD+20, ZXD20b].
carboxylate [OSM20]. carboxylate-promoted [OSM20]. carboxylation
[JMK+20]. Carlo [EG20, GGK20, KCGK20, PFSC20, TIK21]. carrier
[ZHZ+20]. Cartesian [BLB21]. case [AA20, OSHT20, RPD+20a]. CASPT2
[TT20]. CASSCF [Sts20]. catalysis [JRS20]. catalyst [CJH21].
catalytic [CJH21, YFS20, ZMH+21]. catalyzed [HYA+20, PRH20].
Cation [LI20, ODL20]. cations [APR21]. CATKINAS [CJH21]. Cavity
[GRN20]. CBS [CSWW20, Dor20, SK20]. CC3 [GGK20]. CC3-R [GGK20].
CCSD [CS20, CSWW20, Dor20, PRF20]. CCSDT [SK20]. Cd [JS21].
Celebrating [IBL20]. cells [AYO20, S7Z+20]. CEPA/1 [Sän20]. CH
constant [LGM20, dCVARN20]. constrained [MWK+20].
constraints [PDL+21]. construction [HC21, WMZJ20, ZFRM20]. Contact
[CLS+20]. Contacts [MKSS20]. containing [CTBB20, NST+20, ZGZ+20].
continuous [MSS20]. Continuum [BBK20, ALA20, STR20, UB20].
contracted [SM20]. contribution [AK20, Sán20]. convergence [MT20b].
converting [VAP+21]. cooperativity [AK20]. Coordinate [AD20].
coordinates [BLB20]. Coordination [MVP+20, CVGVN+20]. Core
[NRH+20, Pil20]. Core-Substituted [NRH+20]. corrected
[AS21, CTBB20, HCS+20]. Correcting [OLP+20]. correction [ASW20].
correction-scaling [ASW20]. Correcting [OLP+20]. correlogram [ASW20].
corrective [ASW20]. COSMO [VAL20]. COSMO-RS
[VAL20]. cosolvent [TTH+21a]. costly [CSWW20]. Coulomb [CQSG20].
coumarin [ZRSST20]. coumarin-schiff [ZRSST20]. Countrieron [SLR+20].
counterparts [NG20]. Coupled
[BWM20, BSF20, FB21, RCC+20, WGKG20, XCJ20]. coupled-cluster
[BSF20]. coupling [ABZ20b, DZL+20, FCPG20]. couplings [SCKH21].
COV [ONA+20]. Covalent [AWID+20]. Cover [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, Ano20q, Ano20r, Ano20s, BBCT+21b, KFTB20a, RP+20b, SWM+20a, TTH+21b, VV20a]. Cp
[SB20, MT20b]. cross [ABZ20b, ALA20, dBCdL20]. cross-coupling
[MH20, AD20, SPSSH20]. cube [Bal20b]. cupric [XZZ+20]. Current
[BLS20]. Current-Flow [BLS20]. cutoff [DO20]. cycle [Dor20]. cyclization
[TYZ20]. cyclopropane [WG20]. cyclotrimerization [ZMH+21]. D
[PSM+20, SS20, TPZ+20, dCVARN20]. D4 [NG20]. D614G [ONA+20].
Data [SK20, XZ20]. databases [LG2+20]. DD [CD20]. DD-peptidase
[CD20]. deacylation [CD20]. deal [DWSX20]. decomposition
[AV20, AK20, MT20b]. decomposition-based [MT20b]. decorporation
[SDK20]. Deep [LPP20]. DEER [QLC+20]. defective [PSM+20]. defects
[CTBB20, GPEK+20]. Deformation [FMFG20, RA20]. dehydration
[BBK20, CWZD20, FMFG20, RA20, SK20, YXGZ20, APS20, AS21, BWS20, BSF20, BBK+21, CPG21, CQSG20, CTBB20, DZL+20, EPT21, FB20, HCS+20, IYI+20, MWK+20, MH20, MSS20, NG20, NEG+20, NN20, OE20, OMC+20, RCC+20, SDK20, SWF+20, SSYB+20, SZP+20, TT20, VV20b, WKCP21, dBCdL20]. density-fitted [BSF20]. density-functional
[BWS20, NEG+20]. Depend [BWM20]. Dependence [XGZZ20, MH20].
[YXGZ20, CPG21, FB20, IYI+20, JRS20, MSS20, Ngo21, OMC+20, XAD20]. deposited [VTdlM20]. Derivation [FMFG20]. Derivatives [GRN20].
describe [IK21]. Description [BLP20, HRT+20, XCJ20]. descriptors
[GJMPVR+20, HBT+20, LGM20, NTK21]. Design [PAS+20, ZZG+21].
designs [YBS+20], details [TYZ20]. Determination [NNT+20, FKT21].
determines [HYA+20]. Determining [WZZ+20]. deterministic [TS21].

Development [WSL+20], devices [AMF+20]. DFT
[AK20, CS20, FV20, JMV21, LCC+21, MPOC21, NG20, SVDS21, SB20,
WD20, WS21, ZRSST20, ZDBZ20]. DFT-D4 [NG20]. DFT/MRCI
[ZRSST20]. diagnostic [SD21]. diagonalization [MB21].
diagonalization-free [MB21]. diagrams [VFCG20]. diatomic [AA20]. dichalcogenide [PSM+20].
dichromium [MVP+20], dicopper [MVP+20]. Diels
[MNZGO+20, SSYB+20], different [DO20, DWSX20, Sts20, WS21].
differential [SD21], diffusion [PFSC20, RGGD21]. Diimides [NRH+20].
diketones [AV20]. dimensional [STB+20, YAO20], dimer [JC20].
Dimerization [WGKG20]. Dioxide [SB20, ZSD+20], dipole
[BSF20, HPG20]. Direct [FMFG20, YW20]. Directing [AD20]. directions
[YAO20]. Disentanglement [CB20]. disparity [DWSX20]. dispersion
[CTBB20]. dispersion-corrected [CTBB20]. displacement [CB20].
disruption [MTO+20], distance [QLC+20]. Distributed [GJMPVR+20].
distribution [QLC+20], distributions [SKKK20]. Divalent
[PAS+20]. divide [FKT21, NN20]. divide-and-conquer [FKT21, NN20]. DLPNO
[CS20, Dor20, PRF20, Sán20], DLPNO-CCSD [CS20, Dor20, PRF20].
DLPNO-CEPA [Sán20]. DLPNO-CEPA/1 [Sán20]. DNA
[FVSS20, HKSW20]. do [CPG21, GUCC20, ZGZC20]. Dock [Min20].
Docking [XZ20, BAO+20], dodecahedrane [JC20]. DOI [MT20a].
Domain [PT20, PW20]. Domain-based [PW20]. donation [GAG20].
dopamine [TPZ+20], doped [DZL+20, ZDBZ20]. Double
[FV20, OMC+20, CPG21]. Doubles [HFPS20], downregulation [CSP20].
drive [RLR+20]. driven [AV20, SSS+20b]. Drude [KYM20, LJ20, ODL20].
drugs [HBM+20, NST+20, PRH20]. Dual [YW20]. Dual-hybrid [YW20].
due [OLP+20]. dynamic [BAO+20, MPOC21]. dynamically [MT20b].

Dynamics
[FMFG20, HHL+20, KUNT20, YXGZ20, Zac20, BAO+20, CSP20, GGK20,
JRS20, JKK+21, LL21, LKM20, MN20, MAP+20, NN20, OSHT20, PDL+21,
QLC+20, RGGD21, RPD+20a, SPSH20, SKKK20, WSV20, ZFRM20].

E-fields [AMF+20], E4 [WS21]. Effect [AD20, GRN20, JC20, CBF+20,
DO20, FVSS20, JMK+20, PRH20, Sts20, SCZ+21], effective
[BBC+21a, UB20]. Effects
[JDZ+20, SLR+20, SGT+20, GAG20, dCVARN20]. Efficient
[CSGVF+20, MN20, MT20b, EK20a, ZZG+21]. elacestrant [CSP20].
Electric [SHM+20]. electride [DSC20]. electrocatalysts [AR20].
electrolytes [EG20]. electron
[BBC+21a, EPT21, RCC+20, RNP20, SS20, SPSH20, SSO+20, dBCdL20].
Electronic [DGSB+20, SCKH21, TT20, AMF+20, IK21, JMV21, MNZGO+20, OSHT20, PSM+20, RCC+20, SGT+20, STB+20, TPZ+20].
electrophilicities [HBT+20], electrostatic
[AS20, MMK+20, ÖLP+20, UB20]. Electrostatics [HRT+20]. elementary
[DGSB+20]. Elementometalation [WLZM20]. elements [RNP20].
Elongation [MMK+20]. Elucidating [NST+20]. elucidation [HRTSS+20].
eMBED [DGSB+20, MMK+20, UB20]. embrittlement [ZFRM20].
emission [AS20, FB20]. Empirical [LJ20, PWX+20]. Encapsulation
[CBF+20, DSC20]. Encoding [GJMPB+20]. End [MXM20]. End-Point
[MXM20]. energetic [JMV21]. Energetics [HHL+20, NG20, WGKG20].
Energies [BBK20, FMFG20, HFPS20, MFC20, NRH+20, HCS+20, LCC+21, NTK21, ÖLP+20, PRF20, PFSC20, TTT+21]. Energy
[FKT21, GRN20, LPP20, MXM20, Min20, NNT+20, SZLD20, YYS20, AV20, AK20, AA20, BBC20, BBC+21a, CSGVF+20, CSWW20, CSP20, GBM20, HBM+20, KFTB20b, MN20, MSL+20, NTK21, NMFI21, OKI+21, Sán20, SSS+20a, Sts20, TM20, YBS+20]. Energy-based [FKT21]. engineering
[ZFRM20]. Enhanced [FMFG20, DWSX20, LGC21, MH20, ONA+20].
ensemble [HBM+20, QLC+20]. enter [APS20]. enthalpies [Dor20]. Enumeration
[ZLY+20]. Enumeration [SZLD20]. environment [KCF+20]. Enzymatic
[SHM+20, PRF20]. enzyme [DPSG20]. equations [MB21, MT20a].
equatorial [SVDS21]. equilibria [CM20a]. Erratum [MT20a]. establish
europium [HRTSS+20]. Evaluation [PRH20, VAL20, Gao20, SSS+20a].
events [RLR+20]. Evolution [MM20, CG20, YYS20]. Ewald [YLZ+20].
Exchange [BBK20, AA20, SEZ20, VV20b, YW20]. exchange-correlation
[AA20]. Excitation [HFPS20, HCS+20, NRH+20]. Excited
[AIV20, CG20, CPG21, FB21, Gie21, IK21, KL20, OSHT20, OMC+20, RDS+20, Sts20, WD20, ZRSST20]. Excited-state
[AIV20, WD20, ZRSST20]. Exhaustive [BAO+20, SZLD20]. experimental
[HBT+20]. explicit [RPD+20a]. explicit-implicit [RPD+20a]. Exploration
[OYY20, OKI+21, SDK20]. Exploring [MSL+20, NTK21]. expressed
[HCS+20]. Extended [GX20, RGGD21, DWSX20, KGD+21]. Extension
[AY20]. extrapolation [SCKH21]. extremely [JKK+21].

F [APR21, GGK20]. Facilitates [VDK+20]. Facilitating [Zac20].
facilitator [QLC+20]. Factors [AD20]. fail [JRS20]. fail-safe [JRS20].
families [FR21]. Fast [YAO20, AYO20, MSS20, YLY+20]. Fe
[IK21, ZFRM20]. Fe-C [ZFRM20]. Features [SHM+20]. featuring
[ZH+21]. FePS [EK20b]. FePSe [EK20c]. Fermi [AS20]. ferrocenium
[CS20]. FFLUX [HBT+20, KSP21]. FFFParam [KY20]. FGFR3
[MKSS20]. FH [TTT+21]. Field
[BAC20, LJ20, WSL+20, FYSS20, KYM20, MT21, ODL20, PLP+20, SPSH20].

Fitting [AD20, CQSG20, MSS20]. Five [AD20, HGF20, PLP+20].

Five-Coordinate [AD20], five-site [PLP+20], fixed [PLP+20].


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, MXX20, Min20, NNT+20, SLLD20, CSP20, HBM+20, MN20, OL+20, TM20, TYZ20, YBS+20, YIO20].


H [LR20, WSV20, OKI\textsuperscript{+21}, YYS20, dCVARN20]. H/D [dCVARN20]. halide [APR21]. halogen [CB20]. Hamiltonian [IK21]. Hartree [BBK20]. HCVpred [MPuS\textsuperscript{+20}]. heat [BAO\textsuperscript{+20}, SSYB\textsuperscript{+20}]. heat-shock [BAO\textsuperscript{+20}].

Hedgehog [Ban20]. helical [SSS\textsuperscript{+20b}]. helices [VCL20]. helium [BGS\textsuperscript{+20}].

Helix [MKSS20]. heme [SWF\textsuperscript{+20}, SWM\textsuperscript{+20b}]. hepatitis [MPuS\textsuperscript{+20}]. heterobimetallic [ZMH\textsuperscript{+21}]. heterointerface [SZP\textsuperscript{+20}]. Heterolytic [LR20]. heterostructures [PSM\textsuperscript{+20}]. Hf [DBE20]. Hg [SSS\textsuperscript{+20a}].


Homolytic [LR20]. HOPO [SDK20]. Hopping [YXGZ20, FCPG20]. host [BRNB21, GBM20]. host-guest [BRNB21, GBM20]. hot [KSRB\textsuperscript{+21}]. huge [JKK\textsuperscript{+21}]. Human [KUNT20]. hybrid [AR20, FV20, MN20, NG20, RPDE20a, SS20, SZP\textsuperscript{+20}, YW20]. hybrids [CPG21, OMC\textsuperscript{+20}]. hydrated [YC20]. hydration [YIO20]. Hydrides [PWW20]. Hydrocyanation [JFZ\textsuperscript{+20}]. hydrogen [AV20, CVGVN\textsuperscript{+20}, CB20, NTK21, SD21, TTT\textsuperscript{+21}, ZFRM20]. hydrogenation [ZGZ\textsuperscript{+21}]. Hydrostatic [SL20]. hydroxychromones [AIV20]. hydroxylation [HYA\textsuperscript{+20}]. hydroxyquinolinato [AS20].

Hypercube [Bal20a]. Hyperplanes [Bal20a]. hypervalent [SCZ\textsuperscript{+21}].

identified [SSYB\textsuperscript{+20}]. Identifying [PAS\textsuperscript{+20}]. II [ABZ20b, AD20, SVDS21, SSS\textsuperscript{+20a}, YYS20]. III [AS20, HRTSS\textsuperscript{+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, Ano20q, Ano20r, Ano20s, BBC\textsuperscript{+21b}, KFTB20a, RPDE20b, SWM\textsuperscript{+20a}, TTH\textsuperscript{+21b}, VV20a]. imino [YFS20]. immersive [MSL\textsuperscript{+20}]. Immunodeficiency [KUNT20]. impact [SPSH20]. Implementation [YLFZ\textsuperscript{+20}, CSGVF\textsuperscript{+20}, CPG21, OMC\textsuperscript{+20}]. implications [KSP21]. Implicit [GCL\textsuperscript{+20}, RPDE20a]. Importance [HKSW20]. improbable [LR20]. Improved [BBK20, LJ20]. Improving [FB20, SZP\textsuperscript{+20}]. incorporating [Gie21]. increase [LKM20]. increases [HREvdK\textsuperscript{+20}]. independent [LGC21]. Indexes [WZZ\textsuperscript{+20}]. individual [BRNB21]. INDO [Gie21]. INDO/S [Gie21]. Induced [QB20, EK20b, EK20c, FVSS20, TTH\textsuperscript{+21a}]. Influence [GAG20, SVDS21].
[PPSP20, SVDS21].

J [MT20a], jcc.25747 [MT20a], Jones [SG20].

Key [VV20b], kinematic [HC21], kinetic [EG20, JMK+20, dCVAR20], Kinetics [SK20, CD20, DWSX20], Kohn [EK20a, HCS+20, MB21], Koopmans [GX20].

L [OSM20], L-lactide [OSM20], L536S [CSP20], lactamase [KGD+21], lactide [OSM20], landscape [BBC20, YYS20], Laplacian [TTDT20], Large [MFC20, CJWT21], large-scale [CJWT21], Large-Sized [MFC20], Late [PWW20], lattice [NMFI21], layered [EK20c], Leading [AD20, NG20].

leapfrog [MIP+21], Learning [LPP20, HBT+20, YFS20], length [MVP+20], Lennard [SG20], Lennard-Jones [SG20], less [CSWW20], level [BSF20, PHS+20], Lewis [OE20], library [RDS+20, VAP+21], Lif [VDK+20], Ligand [Ban20, JFZ+20, MXM20, NNT+20, AAc20, HGF20, IK21, Ngo21, OLP+20, YIO20], Ligand-Binding [NNT+20, HGF20, Ngo21], ligand-free [YIO20], Ligands [Min20, SZLD20, SVDS21], limit [CVGVN+20, SCKH21], linear [SNN+21], LIO [SDK20]. Lipase [VDK+20], lipid [KFTB20b], liquids [KGD+21], liquid [SPSH20], Liquids [VAL20], lithium [SGT+20], LOBSTER [NEG+20], Local [NEG+20, WSV20, FB21, PW20, VV20b], Lone [TTDT20], Long [BBK20, AS20, HCS+20], Long-range [BBK20, AS20, HCS+20], low [IK21], low-lying [IK21], Löwdin [ASW20], lutidine [TYZ20], lying [IK21].

M [AS20, MH20, ZMH+21, AS20, MH20, ZMH+21], machine [HBT+20, YFS20], Macroscale [HZG+20], magnesium [ZDBZ20], Mannose [KUNT20], many [KSP21], many-body [KSP21], Map [CLS+20], mapping [TTDT20], Martini [MT20a, MT21, BAC20, MT19]. Massively [BBK+21], material [GGK20, SGT+20], materials [ZGZ+20], Mathematical [QB20], Matrix [BLP20, BBB21, RA20, TT20, WMZ20], matrix-product [WMZ20], McConst [SKS21], MD [SSS+20a], MDMS [Zac20], Me [SDK20, WLZM20], Me-3 [SDK20], means [HRTSS+20], measure [AA20], Mechanical [SL20, AAc20, GPEK+20, HKSW20, MMK+20, PWX+20, SPSH20].

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