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Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA

Tel: +1 801 581 5254
FAX: +1 801 581 4148

E-mail: beebe@math.utah.edu, beebe@acm.org, beebe@computer.org (Internet)
WWW URL: <https://www.math.utah.edu/~beebe/>

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Title word cross-reference

(n, n) [BW22a]. $(n \leq 10)$ [YOCMA23]. 1 [Pan23]. 16 [WMJ⁺22]. $1 \leq N \leq 6$ [MPOC21]. 2 [DF22, PSM⁺20, SLMA21]. 20 [Wan23]. 3 [TT20, WKL22]. 4 [SS20]. 4*H* [MSE⁺21]. 5 [AS20, JMV21, SDK20, VTdlM20]. 7 [MdSJ⁺23]. 8 [Bal20b]. [3 + 2] [BAM⁺24, SMB⁺23]. + [APR21, CWZD20, GJL21, KM24, LR20, LEP⁺21, MAM⁺23, OM22, WSV20, YMSS23]. - [Tze21, WSV20, WMJ⁺22]. ¹ [ZHHS21]. ¹³ [KWX23, MCD22, ZHHS21]. ¹⁹ [Ben22, MPV22]. ² [AKN⁺20]. ²⁺ [ALA⁺22, HSG21, IK21, JRS20, MAKZ23, SPSH20, ZRSST20]. ²⁰⁵ [Sai23]. ³ [ERVN24, Mar21, TTDT20]. ³¹ [CMG⁺24, FBP⁺22]. ³ Π_u [Kop22a]. ³ Σ_g^- [Kop22a]. ^{β} [LL21b]. ^{*I*} [PAS⁺20]. ^{*II*} [ĆPP⁺22]. ^{pro} [PPP21]. ^{tz} [BVGB23]. ¹ [Dor20, ERVN24]. ^{$+,0,-$} _{1,2,3} [JX24]. ¹⁰ [LR20, LXP⁺22]. ^{$+$} ₁₂ [PGP⁺23]. ¹⁸ [PP23]. ² [AQRA⁺23, AQMM⁺23, AQIS⁺24, AMM22, ABAQ⁺23, AR20, AWK⁺23, BR23, DSC20, DBE20, DLH⁺23, DGSB⁺20, FP22, FP23, GGK20, GKA⁺23b,

JAP⁺²⁴, KPTT21, LHC⁺²¹, LZW⁺²³, MH20, MC24, MBBU23, MMAZ⁺²³, MK22b, OKI⁺²¹, PTP23, PLT24, RC22, SSSA23, SWF⁺²⁰, SWM^{+20b}, SVTK⁺²², SVR⁺²⁴, SKKG22, dSSRVdM24, SBB⁺²², SLML24, TTK23, TYZ20, TPZ⁺²⁰, TZS⁺²², VTdlM20, VCRP23, WTST24a, WP20, WLZM20, Wan23, XLW⁺²², YYS20, YYZ⁺²¹, ZDBZ20, ZHG⁺²⁴. $\frac{+}{2,3} \frac{0,-}{-}$ [JX24]. $\frac{0,\pm 1,\pm 2}{24}$ [LR20]. $\frac{q}{27}$ [MIP⁺²¹]. $\frac{+}{2}$ [NSKN21]. $\frac{+}{2}$ [GJL21]. $\frac{-}{2}$ [SLR⁺²⁰]. $\frac{-/0}{2}$ [DC22a]. $\frac{3}{3}$ [AMM22, AWK⁺²³, BBL⁺²², EK20b, EK20c, IK21, KPTT21, LM24, LLS^{+22b}, LZW⁺²³, OE20, PTP23, PGP⁺²³, SVTK⁺²², SLR⁺²⁰, SM22b, SCC⁺²², SL20, TAB⁺²⁴, WLZM20, XZW⁺²¹, YMSS23, dCVARN20]. $\frac{4}{4}$ [AMM22, KGS⁺²², LJW⁺²³, MK22b, SM22b, WW24, ZHG⁺²⁴, ZXD20b, ZXD20a]. $\frac{450}{450}$ [HYA⁺²⁰]. $\frac{5}{5}$ [GJL21, HSG21, OKI⁺²¹]. $\frac{6}{6}$ [AQRA⁺²³, AQMM⁺²³, AQIS⁺²⁴, ABAQ⁺²³, ZWL^{+24a}]. $\frac{60}{60}$ [DSC20, HSG21, YLZ⁺²²]. $\frac{80}{80}$ [VKSS24]. $\frac{9}{9}$ [PGP⁺²³]. $\frac{a}{a}$ [PWW20]. $\frac{N}{N}$ [GCP22, MPOC21, SLR⁺²⁰, GPM21b, KPTT21, LWC⁺²⁴, VTdlM20, WMJ⁺²², WZW⁺²⁴, YOCMA23]. $\frac{-}{n}$ [WMJ⁺²², Wan23]. $\frac{-/0/+}{n}$ [TT20]. $\frac{Q}{n}$ [ZDBZ20]. $\frac{\text{spiro}}{\text{spiro}}$ [DK23]. $\frac{x}{x}$ [JS21]. $\frac{+}{y}$ [JS21]. $\frac{\alpha}{\alpha}$ [CSP20, DC22b, SSS^{+20b}]. $\frac{\beta}{\beta}$ [AV20, BPDG21, IAS⁺²⁴, KGD⁺²¹, Mon24, XIV⁺²⁴, ZZ23b]. $\frac{\cdot}{\cdot}$ [AMM22, OE20, OE20]. $\frac{\cdot \cdot \cdot}{\cdot \cdot \cdot}$ [BdLC21, KPTT21, TTT⁺²¹]. $\frac{d}{d}$ [IK21, MSE⁺²¹]. $\frac{d^{10}}{d^{10}}$ [PTP23]. $\frac{D_{9h}}{D_{9h}}$ [PP23]. $\frac{\Delta}{\Delta}$ [EK20a]. $\frac{E_{\text{Lab}} = 0.1}{E_{\text{Lab}} = 0.1}$ [KM24]. $\frac{\eta^1}{\eta^1}$ [LZW⁺²³]. $\frac{\eta^5}{\eta^5}$ [AS23, HSG21]. $\frac{f}{f}$ [SCZ⁺²¹]. $\frac{\gamma}{\gamma}$ [FLT23, KZJ21]. $\frac{H}{H}$ [MIP⁺²²]. $\frac{i}{i}$ [SLML24]. $\frac{K_a}{K_a}$ [SHHH22]. $\frac{\lambda}{\lambda}$ [Ngo21]. $\frac{\log P}{\log P}$ [DHD21, SHH^{+23b}]. $\frac{M}{M}$ [SM22b]. $\frac{\mu}{\mu}$ [MVP⁺²⁰, SLML24]. $\frac{\mu_2}{\mu_2}$ [KBHG23]. $\frac{N}{N}$ [BAM⁺²⁴, DOT22, LWC⁺²⁴, MdSJ⁺²³, NS22, OM22, PFPD21, SHH^{+23b}, WZW⁺²⁴]. $\frac{n = 1}{n = 1}$ [MdSJ⁺²³, TT20, VTdlM20]. $\frac{n = 15}{n = 15}$ [Wan23]. $\frac{n = 3}{n = 3}$ [WMJ⁺²²]. $\frac{o}{o}$ [SHH⁺²⁴]. $\frac{p}{p}$ [AR20]. $\frac{\pi}{\pi}$ [AV20, CMO⁺²⁴, CBF⁺²⁰, FDD⁺²³, LJ20, MP23, ODL20, RTB23, Sch22a, SJZ⁺²¹, TLD⁺²², ZBH⁺²³]. $\frac{q = 1, 0, -1}{q = 1, 0, -1}$ [NSKN21]. $\frac{S}{S}$ [SVTK⁺²²]. $\frac{\sigma}{\sigma}$ [AV20, BKM21, DZ23, JGGPN21, LK22, MP23, RZS⁺²³]. $\frac{sp^2}{sp^2}$ [IW23, NUK21]. $\frac{sp^3}{sp^3}$ [NUK21]. $\frac{\Theta\Phi}{\Theta\Phi}$ [TPD21]. $\frac{U}{U}$ [POPGS22]. $\frac{v = 1, j = 0}{v = 1, j = 0}$ [BBY⁺²¹]. $\frac{Z}{Z}$ [ARR22b, WHJM23].

-1 [ZDBZ20]. **-3-3'-diol** [BBBP⁺²³]. **-acceptor** [JGdC⁺²³]. **-acenes** [MdSJ⁺²³]. **-acetato** [MVP⁺²⁰]. **-alanine** [DC22b]. **-alkanes** [PFPD21]. **-aminotetrazole** [JMV21]. **-aromatic** [RTB23]. **-Azacryptand** [Ari24]. **-Based** [DBE20]. **-benzoquinone** [SHH⁺²⁴]. **-benzyl** [BAM⁺²⁴]. **-block** [AR20]. **-bridged** [KBHG23]. **-C** [HSG21, LZW⁺²³]. **-catalyzed** [HCY⁺²², LLS^{+22b}]. **-complexes** [BKM21]. **-conjugated** [CBF⁺²⁰]. **-Conjugation** [CMO⁺²⁴]. **-covalency** [ZBH⁺²³]. **-Cp** [HSG21]. **-cube** [Bal20b]. **-cyclodextrin** [IAS⁺²⁴]. **-cyclopenta** [MSE⁺²¹]. **-D-Glucopyranose-silver** [Mon24]. **-dependent** [Ngo21, JRS20]. **-diaqua** [MVP⁺²⁰]. **-diketones** [AV20]. **-elimination** [KZJ21]. **-F12** [CK22]. **-functions** [SCZ⁺²¹]. **-grasp** [BPDG21]. **-hairpin** [ZZ23b]. **-helical** [SSS^{+20b}]. **-hexane** [NS22]. **-Hole** [RZS⁺²³, JGGPN21, LK22, Sch22a, SJZ⁺²¹]. **-Hydrido** [SLML24]. **-iron-N**

[GKA⁺23b]. [?]KohnEhlert:2020:PPP. **-lactamase** [KGD⁺21]. **-LIO** [SDK20]. **-matrix** [WHJM23]. **-methylide** [SVTK⁺22]. **-modified** [DOT22]. **-octanol-water** [SHH⁺23b]. **-phenyl** [AS20]. **-pyrazine-M** [MH20]. **-pyrido** [MIP⁺22]. **-pyrrolylenones** [ARR22b]. **-radical** [MP23]. **-sextet** [TLD⁺22]. **-sheets** [XIV⁺24]. **-thymine** [SSS⁺20a]. **-TriPip222** [Ari24]. **-water** [VCRP23]. **-xTB** [OM22].

/CBS [CSWW20, Dor20, SK20]. **/H** [WSV20]. **/N** [ZHG⁺24].

1 [CM20b, CBK⁺24, KUNT20, PWX⁺20, Sán20, WCT⁺23]. **1-** [MLGY24]. **1-11** [ZDBZ20]. **1-chloro-3** [BR23]. **1.0** [Che23, XSP⁺23]. **1.2-a** [MIP⁺22]. **10.1002/jcc.25747** [MT20a]. **12** [SMH21]. **1233zd** [BR23]. **1234yf** [BR23]. **19** [SLMA21].

2 [BBBP⁺23, MSE⁺21, dMBdAVdS24, CM20b, EIT⁺21, GCP22, KLZ⁺23, KGD⁺21, ONA⁺20, PDC23, PPP21, PPRS22, RLR⁺20, SLR⁺20, UAC⁺23, YC23]. **2'-bipyridyl** [BBBP⁺23]. **2-body** [KG23]. **2'-disulfanediybis** [MSE⁺21]. **2-ethenediol** [MLGY24]. **2-ethylhexanoate** [BR23]. **2-HOPO** [SDK20]. **2-hydroxymethyl** [MSA22a]. **2-methoxyethyl** [MSA22a]. **2-siloxy-1-propene** [LLS⁺22b]. **2.0** [FPMD23, Kos22, SWLC22]. **20/HMX** [ZG21]. **2D** [POPGS22, PM21]. **2D-surface** [PM21]. **2D/3D** [POPGS22].

3 [BBBP⁺23, GSJ⁺23, VZG⁺24]. **3-cycloaddition** [SVTK⁺22]. **3-D** [GSJ⁺23]. **3-dienes** [BXY⁺24]. **3-tetrafluoro-1-propene** [BR23]. **3-trifluoro-1-nitroprop-1-ene** [SMB⁺23]. **3-trifluoropropene** [BR23]. **31** [dSSRVdM24]. **3D** [CKH23, DF22, HKFT21, POPGS22, YIO20, YYZ⁺21]. **3D-COF** [YYZ⁺21]. **3D-QSAR** [DF22, HKFT21]. **3D-QSAR/MD** [HKFT21]. **3D-RISM** [CKH23, MY24, YIO20].

4-oxo-4 [MIP⁺22]. **4-triazole-3-thione** [KGD⁺21]. **40** [MT20a]. **42** [WG21]. **43** [SCCZ21]. **4polyGraft** [Che23].

6 [BTC24]. **6-dimethylfulvene** [SHH⁺24]. **6-hydroxyquinolinone** [SEBE21]. **6-lutidine** [TYZ20]. **60th** [IBL20]. **66** [FP23].

7 [CM20b]. **74** [ZHG⁺24]. **7D** [Bal20a]. **7D-Hypercube** [Bal20a].

8-hydroxyquinolinato [AS20].

= [AQRA⁺23, AQMM⁺23, AQIS⁺24, ABAQ⁺23, AS20, APR21, GPM21b, HSG21, LZW⁺23, LXP⁺22, LWC⁺24, LJW⁺23, MH20, PTP23, PP23, SS24, SM22b, SCC⁺22, SL20, WTST24a, WZW⁺24, ZDBZ20].

AA [ZWY⁺22]. **Ab-Initio**

[GK24, RZS⁺²³, RPD^{+20a}, BBBP⁺²³, SNN⁺²¹, XSP⁺²³]. **ABCG2** [SHH^{+23a}]. **ABEEM** [LRqG⁺²²]. **Absolute** [SZLD20, CV22]. **Absorption** [AS20, AS21, ABNG22, BBL⁺²², EK20a, KBK⁺²⁴, SNK24b]. **Ac** [LJW⁺²³]. **accelerated** [GVJ⁺²², PPV⁺²¹, RGGD21]. **accelerates** [NAN⁺²³]. **Accelerating** [GCL⁺²⁰, LGC21, WKL22, ABTM22]. **Acceleration** [JKS23]. **acceptor** [JGdC⁺²³, PTP23, TANC23]. **Accessible** [GCL⁺²⁰, VCL20]. **accuracy** [Cha24, KWX23, RMJ21, YFH⁺²¹]. **Accurate** [DKB23, Dor20, ERVN24, LRF⁺²¹, PWX⁺²⁰, PYA24, Ben22, BP22, CSWW20, NDK24, SHH^{+23b}, SHH^{+23a}, WD20]. **ACE2** [KLZ⁺²³]. **acenes** [MdSJ⁺²³]. **acetaldehyde** [LLS^{+22b}]. **acetate2** [MIP⁺²²]. **acetate2-oxo-2-** [MIP⁺²²]. **acetato** [MVP⁺²⁰]. **acetone** [SHHH22]. **acetonitrile** [PT21]. **acetylcholine** [BRNB21]. **acetylcholinesterase** [AR24]. **Acetylene** [OOY20, SVTK⁺²², SVR⁺²⁴, ZMH⁺²¹]. **achirality** [PFP⁺²¹]. **acid** [Brz22, CMD⁺²², FP23, HREvdK⁺²⁰, HPG20, KZJ21, KK22a, KEK23, NMMC21, ODL20, OE20, PRH20, PLZT23, SHHH22, WGKG20]. **acid-catalyzed** [PRH20]. **acid-water** [KEK23]. **acidic** [FM21, KSS21b, KSRB⁺²¹]. **acidities** [Brz22]. **acidity** [MLGY24, PT21]. **acids** [CH23, PT21]. **acrylate** [MSA22a]. **actinide** [SDK20]. **Actinium** [TLS23]. **actinoids** [LJW⁺²³]. **action** [DSS⁺²⁴, SVDS21]. **Activated** [WLZM20, LYX⁺²²]. **Activation** [BWM20, MKSS20, MGCM21, SLR⁺²⁰, ABZ20b, DZL⁺²⁰, FP22, KDMM24, KJV23, LA20, MC24, PRF20, SHP⁺²³, SLML24, WW24, ZYZ24]. **Active** [VDK⁺²⁰, AFR^{+24a}, BBC20, BP22, HL20, RvWH23, TIK21, TZS⁺²², UR23, WS21]. **activities** [MYYS24, YFS20]. **activity** [BHR⁺²¹, KLC⁺²⁴, NAAP21, SS20, DMTR22, ZMH⁺²¹]. **Acylation** [CD20]. **Ad** [FBP⁺²²]. **Ad-MD** [FBP⁺²²]. **adamantane** [SAZ⁺²³]. **adamantane-like** [SAZ⁺²³]. **adapted** [GH22b, GH23, NTK21, OE20, UR23]. **Adaptive** [DZ23, SS23, ZQ24, NSRK21]. **Adatom** [JGSA22]. **additive** [KYM20]. **additivity** [PB20]. **Adenine** [BVGB23]. **adiabaticity** [RCC⁺²⁰]. **adjusted** [GH22a, VV20b]. **adsorbate** [LHB⁺²⁴]. **adsorbate-substrate** [LHB⁺²⁴]. **adsorbates** [KPDB22]. **Adsorption** [GGK20, FP22, FBM⁺²³, JGSA22, SS23, YYZ⁺²¹, ZHG⁺²⁴]. **advance** [SDH23]. **Advances** [DGS24, MR21, MPR22]. **Advancing** [YGG⁺²³]. **advantage** [BPDG21]. **aeruginosa** [VDK⁺²⁰]. **affinities** [PWX⁺²⁰]. **Affinity** [dSBFdAJ20, DC22b, HLV⁺²⁴, KZOV23, NAN⁺²³, Ngo21, NGD22, SW21, TWT⁺²²]. **affinity-selected** [KZOV23]. **affordable** [DKB23]. **Ag** [MH20, DA22, LZW⁺²³, PP23]. **against** [dMBdAVdS24, EIT⁺²¹, SKL23, UAC⁺²³]. **agent** [SDK20]. **agents** [MML⁺²³]. **aggregate** [RDS⁺²⁰]. **aggregates** [TMO⁺²¹]. **Aggregation** [DB23]. **agonist** [BRNB21]. **aided** [KGS⁺²²]. **AIMD** [WW24]. **Al** [AS20]. **alanine** [DC22b, FP23]. **albicans** [ZOD⁺²²]. **Alchemical** [TM20, WFBB22, BF22, GFRNC21, HB21, WdGG24, Min20]. **alcohols** [ZWY⁺²²]. **Alder** [MNZGO⁺²⁰, MGCM21, NMMC21, SSYB⁺²⁰].

aldimines [BSR22]. **aldol** [LLS⁺22b]. **alexandrite** [RCD⁺24]. **AlGDock** [Min20]. **algebra** [GJMPVR⁺20]. **algebraic** [HD21]. **Algorithm** [AiIS⁺21, WSL⁺20, FR21, GKO⁺22, JKK⁺21, KG23, LHH⁺23, MB21, PSB⁺22, RD23, SS20]. **algorithms** [CP23, GWN21, POvG21, RDB23, ZKJ⁺23]. **alignment** [SCC⁺22]. **alkali** [JMV21, ODL20, OM23, OSM20, YMSS23]. **alkali-metal-like** [YMSS23]. **alkalide** [Ari24]. **alkaline** [ZLLL22]. **alkanes** [PFPD21]. **alkylated** [MAP⁺20]. **alkylpyrroles** [ZHHS21]. **Alkyne** [WLZM20]. **Alkynes** [JFZ⁺20, TYZ20]. **All-atom** [PDC23, BUNO22b, LKM20, WGKG20]. **All-electron** [RNP20]. **all-metal** [MAI22]. **all-purpose** [Mar21]. **Allosteric** [BSL20, CDCT21, TXJT23, XIV⁺24]. **alloy** [RDB23]. **along** [CG20, MH22]. **alpha** [PFPD21]. **alpha-amylase** [PFPD21]. **alternative** [KSRKS21]. **Aluminabenzene** [Brz23]. **Aluminabenzene-based** [Brz23]. **aluminum** [BA22, Kop22a, MC24]. **ambimodal** [SHH⁺24]. **AMgF** [SL20]. **amide** [CRT⁺21]. **amination** [DPY⁺22]. **amine** [CCZ23, CRT⁺21, HPG20]. **amino** [CH23, HREvdK⁺20, ODL20]. **aminoborane** [SR23]. **aminotetrazole** [JMV21]. **aminotransferase** [BBC20]. **AMK_Mountain** [ZLLL22]. **ammine** [MLM⁺24]. **Ammonia** [MFC20, MMF⁺24, SPSH20, YOCMA23]. **ammonium** [ODL20]. **AMOEBa** [ALA⁺22, PLP⁺20, WLWR22]. **among** [DWSX20, GFRNC21, KLZ⁺23]. **Amorphous** [XZZ⁺20, HUO23]. **amylase** [PFPD21]. **amyloid** [BVC⁺23]. **analogs** [CBK⁺24, PLZT23, ZS22]. **analogues** [GK24, SJZ⁺21]. **Analyses** [SLR⁺20, AK20, GM22, GKA⁺23b, HTTT23, KZOV23, PL22, SM23, TS21]. **Analysis** [AKR21, AD20, BBSFA22, KUNT20, MAM21, MAI22, MH20, AÅFJ21, Ano24a, BPL⁺22, BdLC21, JGdC⁺23, CMO⁺24, CJHW21, CSP20, CB20, CR24, DGM22, DPY⁺22, ETT21b, ENR⁺24, EK20c, EPT21, HL20, HS23, IAF⁺24, IWN24, IMT⁺21, JMK⁺20, JRS20, KM22, KF24, KS24, LHG⁺23, MDO⁺20, MSA⁺24, MGCM21, dCB23, MT20b, NUK21, NHFS21, NTK21, NEG⁺20, NVBG23, OTZW24, OKK22, RLHG⁺23, RCC⁺20, RA20, SK23, SR23, SPT21, SWLC22, SH23, TSZ⁺21, THH⁺24, YIO20, YMM⁺24, YWGY22, ZGZC20, ZBH⁺23]. **analytic** [BSF20, IN23b]. **Analytical** [IN23a, LL21b, VCL20]. **Analyze** [dSBFdAJ20, MPOC21, ZK23]. **analyzing** [HPG20]. **Anatomy** [LT23]. **angle** [PDL⁺21]. **angular** [BK24, MR21]. **anharmonic** [ETT21b]. **anhydrase** [KI24]. **ANI** [TTK23]. **ANI-ML** [TTK23]. **aniline** [HRTSS⁺20]. **Anion** [LJ20, FDD⁺23, GP21, JWS⁺24, SNK24b, SLML24, XAD20]. **anion-**[FDD⁺23]. **Anion-Ring** [LJ20]. **Anionic** [AK20, PT20, KPKS23]. **anions** [Brz23, GJL21, Tze21, ZWL⁺24a]. **Anisotropic** [GWN21, ZGZ⁺20, AYO20, BS23]. **anisotropy** [SSP23]. **annealing** [PJJL23]. **annulene** [PC21]. **AnO** [LJW⁺23]. **anode** [SGT⁺20]. **anodes** [AFR⁺24a]. **anolytes** [AFR⁺24a]. **anomaly** [XCJ20]. **antagonists** [CM20b]. **anthracene** [MNZGO⁺20]. **Anti** [KUNT20, NPGP23, SVDS21]. **anti-cancer** [SVDS21]. **anti-HIV** [NPGP23]. **Anti-Human** [KUNT20]. **antibacterial** [RPA⁺24]. **antibiotic** [BF22]. **Antibodies** [KUNT20].

anticancer [DSS⁺24, HBM⁺20]. **antiferromagnetic** [Wan23].
antimicrobial [SEBE21]. **antimony** [PT21]. **antioxidants** [KLC⁺24].
antiporter [WSV20]. **antipsychotic** [dCRM21]. **antiretroviral** [CBK⁺24].
antitumor [PRH20]. **any** [dCRM21]. **AOMadillo** [BK24]. **applicability**
 [GH22a, LSP23]. **Application**
 [GJMPB⁺20, KdILC22, MZ21, PJJL23, PHS⁺20, RMBSPJSG24, TM20,
 Tou21, XAD20, AAe20, MLC⁺23, MK22b, SS23, TSR21, YLZ⁺20, YBS⁺20].
Applications [BBC⁺21a, SHM⁺20, AQMM⁺23, AQIS⁺24, CC22, IYI⁺20,
 IRB⁺23, KGS⁺21, KF24, LM24, SIW21, SKS21, SPT21, TAB⁺24, TCS⁺21a].
applied [HBM⁺20, KCGK20, MMF⁺24, PMT⁺22]. **apply** [PDL⁺21].
Applying [dMBdAVdS24]. **Approach**
 [PWW20, SBG20, SB20, ARR22a, ARR22b, AAL21, ASW20, dMBdAVdS24,
 CN21, CBK⁺24, ĆPP⁺22, DGSB⁺20, DOT22, HBT⁺20, IYI⁺20, IRB⁺23,
 JGGPN21, KMR⁺24, KG23, KPHV23, KEK23, LBH⁺22, LL22, LDT⁺22,
 MZMK⁺21, MJS⁺23, MSA22b, NMF121, OSHT20, PW20, RDB23, STR20,
 TAC⁺23, TMO⁺21, TSR21, VCL20, WYC⁺24, YC23]. **approaches**
 [AV20, CGSP24a, GH22a, PCB⁺24]. **approximate** [BSS⁺22, JCMHT22].
approximation [BMT⁺21, CS23, MCP23, NG20, Shi22, VV20b, YW20].
Approximations [HFPS20, BSF20, RC22]. **aprotic** [OM22]. **aptamer**
 [KR23, TM20]. **AQUA** [LGD⁺20]. **AQUA-MER** [LGD⁺20]. **aquation**
 [HBM⁺20]. **Aqueous** [SSYB⁺20, ĆNF23, KK23, KWB24, KTM⁺23,
 LGD⁺20, PDC23, RPD⁺20a, SNK24b, VV21, YC20]. **Archive** [RTB⁺22].
Area [GCL⁺20, VCL20]. **Arene** [KGS⁺21]. **Argentophillic** [EPT21].
argentum [EPT21]. **argon** [NSH23]. **ARGOS** [NSRK21]. **arithmetic**
 [LPF⁺23]. **ArN** [MAM⁺23]. **Aromatic**
 [ZWL⁺24a, APS20, GAP21, MAI22, ODL20, RTB23, TLD⁺22]. **aromaticity**
 [BGPR24, CMO⁺24, DZ23, FMK24]. **art** [BSF20]. **artifacts** [ÖLP⁺20].
Artificial [QB20, KI24, MZ21]. **aryne** [GM22]. **Aspartate** [HPG20, BBC20].
aspects [KZJ22]. **asplatin** [PPSP20]. **assemblies** [GBM20]. **assembly**
 [MAP⁺20, PRH20]. **Assessing** [BOPJ⁺21a, PRF20, MK22a]. **Assessment**
 [AS21, CK22, FB21, POPGS22, RC22, SK20, SB20, PSA⁺23, ZRSST20].
assisted [ARA22, AV20, ARR22b, CRT⁺21, HUUO23, KF24, KGTL21,
 LL21b, LL22, MLC⁺23, RD24, WRBT21]. **association**
 [GBM20, SSS⁺20b, YJZ⁺22]. **astatine** [PHS⁺20]. **astrochemical**
 [MLGY24]. **asymmetric** [HCY⁺22, PRIP24]. **atom**
 [BUNO22b, ĆNF23, DART21, DLH⁺23, GFRNC21, LKM20, LK22, PDC23,
 SaATR24, SHH⁺23a, WMJ⁺22, WGKG20]. **atom-centered** [LK22]. **atomic**
 [AÅFJ21, BP22, EVKL21, KRW⁺24, KWMPR24b, LL21b, MP24, NEG⁺20].
atomicity [NAAP21]. **Atomistic** [GOY20, HZG⁺20, ONA⁺20, SY21, SL20,
 WKD⁺21, FLT23, LGC21, RMS⁺23]. **atomistically** [NP23]. **atomization**
 [GZFSM21, MCP23]. **atoms** [AKN⁺20, AA20, CC22, CSGVF⁺20, DC22a,
 HLV⁺24, JCMHT22, JGGPN21, LGM20, LGM22, LYX⁺22, MSYS23, MC23,
 NTK21, NSH23, OE20, Sch22b, SG20, Wan23]. **atoms-in-molecules**
 [MC23, NTK21]. **attack** [BA24, CRT⁺21]. **attraction** [IN23b]. **attractors**

[KE23b]. **augmented** [NEG⁺20, Pil20]. **auto** [CJHW21]. **auto-analysis** [CJHW21]. **AutoDock** [PNT⁺22]. **automata** [LCLB24]. **Automated** [COK22, CR24, GSD⁺22, WHJM23, ZLLL22, MNBG⁺21, RSHG23, RB22, SSMP23]. **Automatic** [SM22a, FKT21]. **automatically** [APP24]. **Automation** [WLWR22]. **Automotive** [SC23]. **Automatized** [ABNG22, SYS⁺21]. **AutoMeKin2021** [MNBG⁺21]. **auxetic** [MMAZ⁺23]. **auxiliary** [Fed24, MFS22, NSH23, SM22a]. **availability** [RD24]. **available** [TPD21]. **averaged** [TWT⁺22]. **Avoids** [SZLD20]. **aware** [TCS⁺21a]. **axial** [GSJ⁺23, PPFL23]. **Aza-BODIPY** [FB21]. **azabenzenes** [BKM21]. **Azacryptand** [Ari24]. **azide** [XZZ⁺20]. **aziridine** [JAP⁺24]. **Azobenzene** [YXGZ20, YLZ⁺22]. **azobenzene-containing** [YLZ⁺22]. **AzoChignolin** [ZZ23b]. **azomethine** [SMB⁺23].

B [LHC⁺21, PGP⁺23, YMSS23, DZL⁺20, DDSM23, ERVN24, LWC⁺24, MIP⁺21]. **B3LYP** [LRF⁺21, SW21]. **Ba** [AQRA⁺23]. **BaC** [SGSB23]. **Back** [KE23a, GAG20]. **Backbone** [CLS⁺20, OC23, SGGG22, SSS⁺20b, LL21b]. **backbone-driven** [SSS⁺20b]. **balance** [LBH⁺22, SSS⁺20b]. **balanced** [BK22]. **Band** [PGDD24, GAP21, MA23a, MA23b, ZLLL22, LPP20]. **bandgap** [dARW⁺23]. **bands** [Sch22a]. **Bank** [ENR⁺24]. **BAR** [ZK21]. **barriers** [MML⁺23]. **Barshad** [VFCG20]. **base** [DDSM23, HLV⁺24]. **Based** [DBE20, AV20, ARR22a, BPT⁺23, BMA⁺24, BAO⁺20, Ben22, BEKM24, Brz23, CDCT21, CM20a, CP23, CN21, CR24, DC22b, DPY⁺22, DGSB⁺20, EK20a, FP22, FKT21, GJMPVR⁺20, GJMPB⁺20, GRBN21, GLC⁺22, HTTT23, HM21, HGR⁺24, JMV21, KRW⁺24, KWYN23, KGS⁺21, KZOV23, KDKS21, KdILC22, KSRKS21, KDP⁺22, LHH⁺21, LSP23, LWF⁺22, LEP⁺21, LC22, MNZGO⁺20, MKK⁺22, MLG⁺21b, MAKZ23, MT20b, NEG⁺20, OE20, PPV⁺21, PW20, PMT⁺22, PM21, RKC21, RDK⁺22, RSHG23, RCC⁺20, RDB23, SKL23, SBB⁺22, SM20, SD21, SHHH22, TWT⁺22, UR23, UB20, VWP⁺22, VHS⁺24, Vyb23, WZW⁺24, WYC⁺24, XZC⁺24, YLZ⁺20, ZLLL22, ZS22, ZFRM20, dSSCC24]. **bases** [Sch22a]. **basic** [PSW⁺24]. **basicity** [DC22b, GSH23, MLGY24, SGRN24, SW21]. **Basis** [YXGZ20, CM20b, Fed24, GZFSM21, GH22b, GH23, HGR⁺24, IN23b, KM24, LB21, LB22, MFS22, MM24, MCP23, NSH23, RNP20, SLB23, SM22a, SCKH21, SM20, SCCZ21, TAC⁺23, WCT⁺23]. **basis-set** [HGR⁺24, TAC⁺23]. **bath** [CQSG20]. **batteries** [SGT⁺20]. **battery** [Ore24]. **Bayesian** [AVM21, LBH⁺22]. **Bdf1** [ZOD⁺22]. **Be** [ZDBZ20, BTSB22, RD24, SKKG22, YOCMA23, YMSS23]. **BEE** [AKGD24]. **BeH** [MMAZ⁺23]. **Behavior** [NI22, AK20, BR23, KDKS21]. **Bel** [ZXD20b, ZXD20a]. **BeM** [PTP23]. **Benchmark** [DC22b, MLP22, SW21, SC22, AZKM22, CPG21, CS20, DGSB⁺20, NAN⁺23, OMC⁺20, PGH24, dASRHB21]. **Benchmarking** [LSP23, LWC⁺24, MAKZ23, XZ20, RLHG⁺23, SI22]. **beneficial** [BTSB22]. **Benoît** [IBL20]. **bent** [WG20]. **benzaldehyde** [DSK21, NMMC21, SW21]. **benzene** [CMO⁺24, FMK24, NMFI21, RC22, XCJ20, ZS22].

benzene-bridged [ZS22]. **benzoin** [DSB23]. **benzoquinone** [SHH⁺24].
benzothiadiazole [ZWL24b]. **benzyl** [BAM⁺24]. **benzyne** [GM22].
benzyne/aryne [GM22]. **benzynes** [BGPR24]. **Beryllium**
 [MSYS23, Kop22b, PTP23, RMS⁺23, SKKG22, THLC⁺23, ZDBZ20].
beryllium-doped [ZDBZ20]. **best** [KDP⁺22, ZHHS21]. **between**
 [AR24, BW22a, BAM⁺24, CS20, CTBB20, dSCCN21, HYA⁺20, KR23, Klo22,
 KPR23, MML⁺23, MPP23, Min20, NTK21, PTP23, RZS⁺23, SMB⁺23,
 SSS⁺20b, XIV⁺24]. **BFGS** [FR21]. **bias** [KSRB⁺21, Tik23]. **biased**
 [DHN⁺21, RGGD21]. **biased/accelerated** [RGGD21]. **biasing**
 [GVJ⁺22, RR22]. **bidentate** [LLKS23, TLS23]. **bidirectional**
 [MPP23, MMAZ⁺23]. **bifunctional** [HBM⁺20]. **bilayers** [PRIP24]. **bile**
 [WGKG20]. **bileptic** [GPM21b]. **bimetallic** [MAKZ23]. **binary** [MJS⁺23].
BinderSpace [KZOV23]. **Binding**
 [GOY20, KLZ⁺23, KPKS23, MXM20, Min20, NNT⁺20, SZLD20,
 dSBFdAJ20, BRNB21, CSP20, FDD⁺23, GH22a, HGF20, HLV⁺24, IYI⁺20,
 KR23, MAKZ23, MSA22a, NAN⁺23, NTK21, NBE⁺23, Ngo21, NST⁺20,
 NGD22, NN20, ÖLP⁺20, PWX⁺20, RLHG⁺23, SWF⁺20, SWM⁺20b,
 SSO⁺20, TWT⁺22, WKCP21, XZX⁺22, YIO20, ZQ24, ZOD⁺22]. **binuclear**
 [KKAK23]. **bio** [AAID22]. **bio-membranes** [AAID22]. **bioactivity**
 [MPuS⁺20]. **biochemical** [YWGY22]. **bioisosterism** [dMBdAVdS24].
Biological [AWID⁺20, CKH23, CBB⁺21, JKK⁺21, JKS23, SS20]. **biology**
 [FPMD23, IBL20]. **biomacromolecules** [LRKD23]. **biomolecular**
 [MAKZ23]. **Biomolecules** [WZZ⁺20, PGH24, SH23, ZGZC20]. **biophysical**
 [SKS21]. **bioremediation** [FPFD21]. **biosensor** [SPT21]. **biosystems**
 [GUCCR20]. **biphenyl** [BdLC21]. **biphenylene** [RTB23]. **BIPS** [DK23].
bipyridyl [BBBP⁺23]. **birthday** [IBL20]. **bis** [YFS20]. **bishistidyl** [FAK24].
bithiophene [AST24]. **Block** [RA20, AR20, LRKD23]. **blocks** [RA20]. **Blue**
 [HBM⁺20]. **BMP** [CM20b]. **BMP-2** [CM20b]. **BMP-7** [CM20b]. **BN**
 [MdSJ⁺23]. **BN-** [MdSJ⁺23]. **BODIPY** [FB21]. **BODIPY/Aza** [FB21].
BODIPY/Aza-BODIPY [FB21]. **body**
 [BMT23, KG23, KSP21, KWMPR24b, LLZ⁺23, NI22, VWJ23, WFLZ23].
Bohmanian [Tik23]. **Bohmanian-style** [Tik23]. **Boltzmann**
 [BSB⁺24, NSRK21, RCC21, SCvW22, UYJ⁺24, WK21, XAD20]. **Bond**
 [LR20, AV20, ARR22b, AD23, AKGD24, AR24, APR21, BKM21, CRT⁺21,
 DK23, GH22a, HL20, HSG21, MDO⁺20, MLB⁺23, MIP⁺22, MC23, PDL⁺21,
 Sch22b, SSS⁺20a, SJZ⁺21, SHP⁺23, TTT⁺21, XCJ20, ZMH⁺21].
bond-angle [PDL⁺21]. **bond-driven** [AR24]. **bonded**
 [DGM22, LKT21, LML⁺23]. **Bonding**
 [DDSM23, FNPD22, GM22, KE23b, LHG⁺23, MCD22, SMH21, THLC⁺23,
 AV20, AWK⁺23, AA20, BEKM24, BGS⁺20, BCN22, CVGVN⁺20, DGM22,
 JX24, EK20c, FDK22, FAK24, GKA⁺23b, GSJ⁺23, JC20, JGGPN21, KZ24,
 KS24, LLKS23, LXP⁺22, MVP⁺20, MSYS23, MP23, MIP⁺21, NEG⁺20,
 OTZW24, SM23, Tze21, WCD⁺23, YSMS24, ZBH⁺23, dBCdL20]. **bonds**
 [Brz22, CB20, GH22a, HS23, KP TT21, NTK21, PTP23, SGGG22,

dASRHB21, Sch22b, SD21, WG20, ZBH⁺²³]. **Boosting** [KN21]. **borane** [ZZG⁺²¹]. **boranylborane** [PFP⁺²¹]. **Born** [GCL⁺²⁰]. **Boron** [FP22, LWC⁺²⁴, MAI22, NDK24, ZYZ24, ZS22]. **boron-centered** [ZYZ24]. **boron/phosphorus** [ZS22]. **boron/phosphorus-based** [ZS22]. **boronic** [FP23]. **borylene** [DGM22]. **boryne** [KDMM24]. **both** [KCF⁺²⁰, PRH20]. **bottom** [IL24]. **bottom-up** [IL24]. **boundaries** [VZG⁺²⁴]. **boundary** [BSB⁺²⁴, CX21b, PSMPB21, RCC21, SCvW22, YAO20]. **bpy** [IK21]. **Br** [SCC⁺²², ABAQ⁺²³, GGK20, MBBU23]. **Branched** [TPB22]. **breakage** [FVSS20]. **Breakdown** [AD20]. **Breaking** [LR20]. **breathing** [CBF⁺²⁰]. **Breit** [IN23a]. **Breslow** [DSB23]. **brevicompactum** [HYA⁺²⁰]. **bridge** [JGdC⁺²³]. **bridged** [KBHG23, ZS22]. **Bridging** [HZG⁺²⁰, UYJ⁺²⁴, LLKS23]. **Brownian** [LL21a, Shi22]. **Brownian-type** [LL21a]. **BSSE** [LB21, LB22, SLB23]. **BSSE-corrected** [LB21, LB22, SLB23]. **buckle** [GNL⁺²²]. **buckybowls** [FDD⁺²³]. **buffer** [FKT21]. **Building** [AD20, AAID22, LRKD23]. **building-block** [LRKD23]. **bulk** [CX21b, NDK24, TANC23, dARW⁺²³]. **bundle** [NYM22, SIW21].

C [GPM21b, HSG21, LR20, LZW⁺²³, OKI⁺²¹, PP23, ZFRM20, ARR22b, DZL⁺²⁰, DSC20, DK23, GAP21, IAF⁺²⁴, KWX23, MPuS⁺²⁰, MCP23, MCD22, PGP⁺²³, SHP⁺²³, VKSS24, YLZ⁺²², ZHHS21]. **C-NMR** [MCD22]. **C2** [FCB23]. **C22** [FCB23]. **cAAC** [GPM21b]. **Cage** [SSSA23, DSC20, GGK20]. **Cage-size** [SSSA23]. **cages** [AST24]. **CAI** [ZXD20a]. **CAI** [ZXD20b]. **calculate** [FBP⁺²², SS20, WFBB22]. **calculated** [ABAQ⁺²³]. **Calculating** [KWX23]. **Calculation** [CV22, Sán20, Cha24, CSWW20, HNCL24, KM22, MR21, NML21, ÖLP⁺²⁰, PRF20, RB24, SCCZ21, VCL20, VV21, YBS⁺²⁰, ZQ24]. **Calculations** [DBE20, MXM20, Min20, AiIS⁺²¹, BSS⁺²², BSR22, CMG⁺²⁴, CKH23, CLTMd⁺²³, DGsb⁺²⁰, EK20b, EPT21, FV20, FB20, GBM20, HB21, HM21, HRTSS⁺²⁰, HLV⁺²⁴, KL20, KK23, LB21, LB22, LWC⁺²⁴, MLC⁺²³, MAM⁺²³, Mar21, MY24, MSA⁺²⁴, MCD22, NAN⁺²³, PFSC20, QLC⁺²⁰, RH21, SW21, SRB21, SWF⁺²⁰, SWM^{+20b}, SSMP23, SLB23, SZP⁺²⁰, TM20, TT20, UR23, WdGG24]. **Calibration** [DPSG20]. **CAM** [LRF⁺²¹]. **CAM-B3LYP** [LRF⁺²¹]. **camptothecin** [PRH20]. **Can** [BTSB22, RD24, PBM21]. **cancer** [SVDS21]. **Candida** [ZOD⁺²²]. **canonical** [GGK20, KSRB⁺²¹, ZKJ⁺²³]. **capacity** [SKKG22]. **capped** [AST24]. **caps** [Fed24]. **capsanthin** [PSA⁺²³]. **capture** [BBB⁺²³, KOD21]. **carbene** [DGM22, YSMS24]. **carbene-borylene** [DGM22]. **Carbenes** [PAS⁺²⁰, JGSA22, KJV23]. **Carbocyclic** [PAS⁺²⁰]. **carbohydrates** [KB22]. **Carbon** [ZXD20a, APS20, AS21, AKN⁺²⁰, BW22a, BR23, CBF⁺²⁰, CTBB20, DC22a, GPEK⁺²⁰, GKA^{+23b}, IW23, LZW⁺²³, MP23, PGP⁺²¹, RZS⁺²³, ZSD⁺²⁰, ZXD20b]. **carbonic** [KI24]. **carbonyl** [FNP22]. **carboxy** [FDK22]. **carboxy-neuroglobin** [FDK22]. **carboxyl** [CCZ23]. **carboxylate** [OSM20]. **carboxylate-promoted** [OSM20]. **carboxylates** [PCI23]. **carboxylation** [JMK⁺²⁰]. **Carlo** [DMD⁺²¹, EG20, GGK20,

GNL⁺²², KCGK20, KEK23, PFSC20, TIK21, TMO⁺²¹, ZKJ⁺²³].
Carlo/DFT [TMO⁺²¹]. **carrier** [LHC⁺²¹, ZGZ⁺²⁰]. **Cartesian**
 [BLB20, LSCK23]. **Case**
 [ARR22b, AA20, BEKM24, HM21, LWLC21, NPGP23, OSHT20, PDGD23,
 RPD^{+20a}, RCD⁺²⁴, SVR⁺²⁴, TMO⁺²¹, VM23]. **cases** [Ari24]. **CASPT2**
 [TT20]. **Cassandra** [DMD⁺²¹]. **CASSCF** [LJW⁺²³, Sts20]. **catalysis**
 [JRS20]. **catalyst** [CJHW21, MAM21]. **catalysts**
 [DRBT24, DLH⁺²³, MLB⁺²³, MKB⁺²¹, SHP⁺²³, WKG⁺²³]. **catalytic**
 [CJHW21, CL23, DSK21, MKB⁺²¹, MYYS24, PFPD21, PM21, YFS20,
 ZMH⁺²¹]. **Catalyzed**
 [LLS^{+22b}, AMM22, BXY⁺²⁴, HCY⁺²², HYA⁺²⁰, NMMC21, PRH20, SKY24].
cathode [LCP24]. **Cation**
 [LJ20, Kop22b, ODL20, OAN⁺²³, PGP⁺²³, YMSS23, dARW⁺²³]. **cationic**
 [KPKS23]. **cations** [APR21, Jab22a]. **CATKINAS** [CJHW21]. **caused**
 [LML⁺²³]. **Cavity** [GRN20, BBSFA22, MJS⁺²³]. **CBS**
 [CSWW20, Dor20, SK20]. **CC3** [GGK20]. **CC3-R** [GGK20]. **CCI** [KGS⁺²²].
CCSD [CS20, CK22, CSWW20, Dor20, GRBN21, KG23, MLB⁺²³,
 MEKH22, MCP23, PRF20, SI22]. **CCSDT** [SK20]. **Cd** [AQRA⁺²³, JS21].
CdSe [LWLC21]. **Celebrating** [IBL20]. **cells** [AYO20, SZP⁺²⁰, TANC23].
CellSys [AAID22]. **cellular** [LCLB24, YMM⁺²⁴]. **cellular-scale** [YMM⁺²⁴].
cellulose [LGJF22]. **center** [LK22]. **centered** [KZ24, LK22, ZYZ24].
CEPA/1 [Sán20]. **cesium** [GH23]. **CGeGaAl** [DC22a]. **CH**
 [AMM22, SVTK⁺²², dCVARN20, BdLC21, KPTT21, MK22b, SVTK⁺²²,
 SLR⁺²⁰, dSSRVdM24, SCC⁺²², WW24, XZW⁺²¹, ZHG⁺²⁴, dCVARN20].
chain [Shi22, SSS^{+20b}]. **chains** [BSR22, ODL20]. **Chalcogen**
 [MDO⁺²⁰, SaATR24, dASRHB21]. **Chalcogen-mercury** [MDO⁺²⁰].
chalcogenides [EPT21]. **chalcogenuranes** [dSCCN21]. **chalcone**
 [ARR22a]. **challenge** [RLHG⁺²³, RvWH23]. **Challenging**
 [JGGPN21, BOPJ^{+21a}, CTPJH22, UB20, VM23]. **Chalmers** [AÅFJ21].
CHAMPION [AÅFJ21]. **change** [JGM21, XIV⁺²⁴]. **changes**
 [BBSFA22, ÖLP⁺²⁰, TTH^{+21a}]. **changing** [PNT⁺²²]. **channel**
 [CX21b, LA20, XAD20]. **channels** [OKI⁺²¹]. **Chaperone** [VDK⁺²⁰].
chapter [SVR⁺²⁴]. **character** [BGS⁺²⁰, LHG⁺²³, MLX⁺²⁴, SD21].
characteristics [AQRA⁺²³, AQIS⁺²⁴, KZP22, MML⁺²³].
Characterization [BVC⁺²³, PT20, dBCdL20, GPEK⁺²⁰, Kop22a, LZW⁺²³,
 MC23, PGP⁺²¹, PYA24, SBB⁺²²]. **characterize** [APP24, LKK⁺²³].
Charge [GRN20, SKKK20, AST24, Ano24a, BBC^{+21a}, JGdC⁺²³,
 BOPJ^{+21a}, CPG21, CMO⁺²⁴, CB20, CCPR24, IN23b, IK21, KCGK20,
 KWB24, dCB23, NVBG23, ÖLP⁺²⁰, Ore24, OMC⁺²⁰, PLP⁺²⁰, PWX⁺²⁰,
 SPSH20, SK23, SZL23, SHH^{+23a}, XZW⁺²¹, ZWY⁺²², ZGZ⁺²⁰, dCRM21].
charge-scaling [ZWY⁺²²]. **charge-transfer**
 [BBC^{+21a}, BOPJ^{+21a}, CCPR24, IK21]. **charged** [HPG20, SSP23]. **charges**
 [CX21b, LK22, MM24, NEG⁺²⁰]. **Charm** [WMZJ20]. **CHARMM**
 [BTL24, FVSS20, KLP⁺²², KYM20, QLC⁺²⁰, TPB22, VWP⁺²²].

CHARMM-based [VWP⁺22]. **CHARMM-GUI** [KLP⁺22, QLC⁺20].
Chem [MT20a, WG21, CSG⁺21]. **chemcoord** [WHJM23]. **Chemical**
 [AWK⁺23, AWID⁺20, BEKM24, CGMRVBAl22, DF22, MSL⁺20, OoY20,
 PAS⁺20, VAL20, WG21, AKGD24, APR21, BHR⁺21, Ben22, BBK⁺21,
 CKH23, CP23, CSG⁺21, CB20, DGS24, DGsb⁺20, EK20c, HGF20, JAP⁺24,
 KWX23, KFLP21, KB22, LT23, LC22, MLC⁺23, MH22, MN20, MAI22,
 MPV22, NEG⁺20, OKI⁺21, PHS⁺20, Pil20, RSHG23, SBFSJMLU23, SIW21,
 SYS⁺21, SC23, SR23, SKT24, SCC⁺22, TANC23, TTDT20, Tze21, UB20,
 VWJ23, Wan21a, Wan21b, WHJM23, YGG⁺23, ZHHS21].
chemical-bonding [NEG⁺20]. **chemically** [BUNO22b, BP22, TCS⁺21a].
chemicals [CSG⁺21, WRVP22]. **Chemisorption** [PKT21]. **chemistry**
 [BBB⁺23, DKB23, GP21, KRSD⁺23, KBK⁺24, LGM20, NVBG23, PSGL21,
 SDK20, SSMP23, SNN⁺21, TPD21, TLS23, TCS⁺21a, TV22, TSH⁺23,
 VAP⁺21, XSP⁺23]. **chemoselectivity** [SLML24]. **Chignolin** [ZZ23b].
ChimeraX [SIW21]. **chiral**
 [GJMPVR⁺20, MNZGO⁺20, MLX⁺24, PFP⁺21, SRB21]. **chirality**
 [PPFL23]. **chloride** [Mil21]. **chloro** [BR23]. **choice** [SCKH21]. **Cholesterol**
 [Ban20]. **chromophore** [RPD⁺20a]. **chromophores** [BSR22, MSA22b]. **CI**
 [CN21, Gie21, UR23]. **CIFDock** [VWP⁺22]. **circuit** [KF24]. **circular**
 [MSA22b]. **Cis** [YXGZ20]. **Cis-Azobenzene** [YXGZ20]. **Cl**
 [SCC⁺22, ZG21, ABAQ⁺23, BEKM24, GGK20, MBBU23, SLR⁺20, WSV20].
CL-20 [ZG21]. **CL-20/HMX** [ZG21]. **Clar** [TLD⁺22]. **classic** [MAI22].
classical [BdLC21, DHD21, HUUO23, KLP⁺22]. **ClassicalGSG** [DHD21].
classify [DTA21]. **clathrate** [VCRP23]. **clathrate-hydrates** [VCRP23].
cleavage [CRT⁺21, JRS20]. **close** [CGMRVBAl22]. **closed**
 [GSSG24, Klo22, MB21, SM23]. **closed-shell** [GSSG24, Klo22, MB21].
Cluster [BLP20, WZZ⁺20, BtSB22, BSF20, DC22b, FB21, GRBN21,
 HPM⁺21, KPDB22, KTBS23, LWC⁺24, MMF⁺24, NSKN21, SKKG22,
 SAZ⁺23, STR20, WP20, ZWL⁺24a]. **cluster-continuum** [STR20]. **Clusters**
 [MFC20, AD23, AKGD24, BWS20, CVGVN⁺20, DZL⁺20, JS21, KE23b,
 KPTT21, KG23, KEK23, LL21a, LLZ⁺23, LXP⁺22, MAI22, Mil21, NAAP21,
 NI22, NST⁺20, OM22, OM23, POPGS22, RDB23, TT20, TSR21, VTdlM20,
 WMJ⁺22, Wan23, WZW⁺24, XDZ23, YOCMA23, ZDBZ20]. **Cm** [LJW⁺23].
CO [BR23, PTP23, WLZM20, LXP⁺22, DZL⁺20, GKA⁺23b, MSA22a,
 AMM22, AR20, Ano24a, DGsb⁺20, FP22, FP23, FDK22, JAP⁺24, LHC⁺21,
 MC24, MK22b, RC22, SK23, SBB⁺22, SLML24, VCRP23, WP20, XLW⁺22,
 YYZ⁺21, MYYS24]. **co-deposition** [MSA22a]. **co-factor** [GKA⁺23b].
CO-N [XLW⁺22]. **coagulants** [RD24]. **Coarse**
 [MT20a, WSL⁺20, WZZ⁺20, BS23, CST23, GWN21, IL24, KGTL21, LL21b,
 LL22, MT19, SSDL⁺23, XZC⁺24]. **Coarse-Grained**
 [MT20a, WSL⁺20, WZZ⁺20, BS23, CST23, GWN21, IL24, KGTL21, LL21b,
 LL22, MT19, SSDL⁺23]. **coarse-to-fine** [XZC⁺24]. **cobalt** [HCY⁺22].
COBRAMM [ABNG22, CMG⁺24]. **cocrystal** [ZG21]. **Code**
 [SHM⁺20, TS21]. **codelivery** [PRH20]. **codes** [WK21]. **coefficient**

[SHH⁺23b, UKBD23]. **coefficients** [BUNO22b]. **Coelenterazine** [GOY20]. **Coenzyme** [CWZD20]. **COF** [YYZ⁺21]. **coherent** [EVKL21]. **coinage** [FBM⁺23, MCD22, YSMS24]. **Colab** [PSW⁺24]. **coli** [CGSP24a]. **collective** [BPT⁺23]. **collective-variable** [BPT⁺23]. **collision** [BBY⁺21]. **Colorings** [Bal20a]. **combination** [GVJ⁺22, KK23]. **Combined** [RMJ21, AiIS⁺21, KPHV23, LDT⁺22, TIK21, TMO⁺21, WKD⁺21]. **Combining** [BMT⁺21, MKB⁺21, TCS⁺21a, WSL⁺20, KN21, NML21]. **Comment** [MT21, NTK21, WFLZ23, WG21, CPG21, Wan21a]. **common** [MSA22a]. **communications** [AiIS⁺21]. **Comparative** [JMV21, PM21, BA24, SGRN24, THH⁺24]. **compared** [LML⁺23, WD20]. **Comparing** [CCHS23]. **Comparison** [BSS⁺22, CN21, NUK21, RLHG⁺23, SK20, WK21, Ano24a, DGM22, GG22, HSG21, SVTK⁺22, SK23]. **compatible** [BTL24, PLP⁺20]. **competing** [ČNF23]. **competition** [SJZ⁺21]. **complementary** [FPMD23, SM22a]. **Complete** [HL20, DMD⁺21, MCP23, SCKH21]. **Complex** [NGD22, ALA20, AAL21, BF22, GNK⁺23, KL20, LML⁺23, Mon24, OE20, SWF⁺20, SIW21, SC23, TM20, WHJM23, YYS20, ZMH⁺21, ZZG⁺21]. **complexation** [SGRN24, SDK20]. **Complexes** [AD20, BGS⁺20, ASL⁺20, AS23, AS20, Ari24, BKM21, Brz22, CL23, CMD⁺22, ČPP⁺22, DGM22, DSK21, FNP22, GKA⁺23b, GP21, Jab22a, KMR⁺24, KK23, KBHG23, KKAK23, KDP⁺22, LLKS23, LKT21, LZW⁺23, LML⁺23, MNH21, MVP⁺20, MLM⁺24, MGB⁺22, MYYS24, MCD22, NBE⁺23, PTP23, PB20, PLT24, PP23, RLHG⁺23, SVDS21, SEZ20, SD21, THLC⁺23, WYC⁺24, XZX⁺22, YFS20, YSMS24, dBCdL20]. **component** [IWN24, KWYN23, KL20]. **components** [AV20, NTK21]. **composite** [CK22, PW20, PCB⁺24, SFS24]. **composites** [MML⁺23]. **Composition** [YLZ⁺22, JS21]. **Composition-selective** [YLZ⁺22]. **compound** [EK20b, HTFY21, QLW⁺22b, SWM⁺20b]. **compound-protein** [QLW⁺22b].

Compounds
[PAS⁺20, SL20, BW22a, dMBdAVdS24, KBK⁺24, MAI22, MCP23, MP23, NI22, NPGP23, PDGD22, PDGD23, PHS⁺20, QLW⁺22b, SW21, SS24].

Comprehensive [SS24, YIO20, JGdC⁺23, PRH20, ZK23]. **compressed** [XZZ⁺20]. **compression** [CC22]. **Comput** [MT20a, WG21]. **Computation** [ALA20, CM20a, GZFSM21, MN20, SZL23]. **Computational** [ARA22, AD20, AR20, BW22a, ČNF23, GOY20, KZP22, KMR⁺24, KJV23, KBHG23, MPV22, Sai23, SKGG23, XZ20, ZMH⁺21, CGSP24a, CBK⁺24, CRT⁺21, DSS⁺24, JC20, KZJ22, KPHV23, LCP21, MDO⁺20, MK22a, MSA22b, NMMC21, Ore24, PSGL21, SW21, SVDS21, SBB⁺22, TTH⁺21a, VAP⁺21, WG20]. **Computationally** [ZBH⁺23, TPD21]. **Computations** [Bal20a, Bal20b, BSF20, RBM⁺23]. **compute** [SYS⁺21]. **computed** [MEKH22, MM24, ZWR22]. **Computer** [KGS⁺22]. **Computer-aided** [KGS⁺22]. **Computing** [GJMPVR⁺20, IRB⁺23, JKK⁺21, KWMPR24b, MPP23, POvG21].

concentrations [CX21b]. **conceptual** [ČPP⁺22, GD23, MGCM21].

concern [KLZ⁺23, WRVP22]. **concerning** [VTdlM20]. **Concerted** [BBBP⁺23, SBB⁺22]. **condensation** [DSB23]. **condensed** [LWF⁺22, SNK24b]. **condition** [GM22, MT20b, YAO20]. **conditions** [CX21b, FM21, LGJF22, PSMPB21]. **conditions-mechanistic** [LGJF22]. **conductance** [KTM⁺23]. **conducting** [LDT⁺22]. **conductivity** [KTM⁺23, RTB23]. **configuration** [CV22, MR21, MPR22, PHS⁺20, SBD⁺21, UR23, WMZJ20]. **configuration-based** [UR23]. **configuration-interaction** [WMZJ20]. **configuration-space** [SBD⁺21]. **configurational** [BAO⁺20]. **confined** [JC20]. **confinements** [AK20]. **Confining** [VCRP23]. **Conformation** [KK23, DF22]. **Conformational** [DA22, MVV22, OM22, PGH24, TPZ⁺20, FBP⁺22, KN21, OC23, PDC23, PJJL23, SS20, STR20, TTH⁺21a, TZS⁺22, WSV20, XIV⁺24, ZGZC20]. **Conformations** [XZX⁺22, BTC24, KGS⁺22]. **conformer** [JGK⁺22, JGK⁺22]. **Conformer-RL** [JGK⁺22]. **Conformers** [ONC20, PSA⁺23]. **congeners** [POPGS22]. **conical** [AIV20]. **conjugated** [CBF⁺20, FCB23, KZJ22]. **Conjugation** [CMO⁺24]. **connection** [MPV22]. **Conquer** [JGM21, FKT21, NN20, SY21]. **Conquering** [VZG⁺24]. **consequences** [SBD⁺21]. **conservation** [CH23]. **considering** [SAZ⁺23]. **consistent** [CV22, CQSG20, CTPJH22, CR24, IW24, LB21, LB22, NSH23, PW20, SLB23, SKKK20, VWJ23]. **Constant** [SDH23, FNY21, MLM⁺24, SaATR24, SSS⁺20a]. **constants** [LGM20, LGM22, SYS⁺21, dCVARN20]. **constrained** [FNY21, MWK⁺20, TV22]. **constraints** [BMT⁺21, LSCK23, OAC23, PDL⁺21]. **construct** [APP24]. **construction** [HC21, HD21, WMZJ20, ZFRM20]. **Contact** [CLS⁺20]. **Contacts** [MKSS20]. **containing** [CTBB20, DART21, ENR⁺24, NST⁺20, DMTR22, YLZ⁺22, ZGZ⁺20]. **context** [SS23]. **continuous** [MSS20]. **Continuum** [BBK20, ALA20, PCI23, SJA24, STR20, UB20, VL22]. **contracted** [SM20]. **contributing** [CH23]. **contribution** [AK20, Sán20]. **contributions** [VWJ23]. **control** [AR24, DYGM21]. **controlled** [CGMRVBAl22, FR21]. **controlling** [SLML24]. **controls** [dARW⁺23]. **conventional** [SGGG22]. **convergence** [CMG⁺24, MT20b]. **conversion** [FP23]. **converting** [VAP⁺21]. **convolution** [WCY⁺24]. **cooperativity** [AK20, KS24, SJZ⁺21]. **Coordinate** [AD20, BCN22, dSCCN21, PBM21]. **coordinates** [ABTM22, BLB20, LL21b, WHJM23]. **coordinating** [Brz23]. **Coordination** [MVP⁺20, YMSS23, Ano24a, CVGVN⁺20, SK23, TLS23]. **copolymer** [LEP⁺21]. **copolymer/ionic** [LEP⁺21]. **copolymers** [BSR22]. **copper** [RLHG⁺23]. **cordierite** [RCD⁺24]. **Core** [NRH⁺20, HMK23, HNCL24, MCP23, PDGD23, Pil20, SAZ⁺23]. **Core-Substituted** [NRH⁺20]. **correct** [HMK23]. **corrected** [AS21, CHVF21, CTBB20, GAP21, HCS⁺20, KDLP21, LB21, LB22, SLB23]. **Correcting** [ÖLP⁺20, Ore24]. **Correction**

[Ano24a, ASW20, BJ22, DYGM21, HGR⁺²⁴, NI22, VL22].
correction-scaling [ASW20]. **Corrections** [HFPS20, POPGS22].
correlated [SM22a]. **Correlation** [NSH23, AA20, HM21, MH22, MPR22, MM24, NTK21, PW20, RMJ21, Sán20, SPSH20, SSO⁺²⁰, TV22].
correlations [AS20, YW20]. **corresponding** [HSG21]. **corrole** [ASL⁺²⁰].
COSMO [GSH23, SHHH22, VAL20]. **COSMO-RS** [SHHH22, VAL20].
cosolvent [TTH^{+21a}]. **cost** [CK22, DKB23, KWX23]. **costly** [CSWW20].
Coulomb [CQSG20]. **coumarin** [ZRSST20]. **coumarin-schiff** [ZRSST20].
Counterion [SLR⁺²⁰, LCLB24]. **counterparts** [NG20]. **counterpoise** [NI22].
Coupled [BWM20, BS23, BTSB22, BSF20, ČNF23, DC22b, FB21, GRBN21, HPM⁺²¹, RCC⁺²⁰, RDB23, WGKG20, WdGG24, XCJ20].
coupled-cluster [BSF20, DC22b]. **Coupling** [BSB⁺²⁴, ABZ20b, AMM22, DZL⁺²⁰, FCPG20, HCY⁺²², IMT⁺²¹, MML⁺²³, POPGS22, Tou21, Wan23].
couplings [SBD⁺²¹, SCKH21]. **COV** [ONA⁺²⁰, dMBdAVdS24, EIT⁺²¹, KLZ⁺²³, PDC23, PPP21, PPRS22, SLMA21, YC23, UAC⁺²³]. **CoV-2** [UAC⁺²³].
covalency [ZBH⁺²³]. **Covalent** [AWID⁺²⁰, GSJ⁺²³, SKT24].
Cover [AFR^{+24b}, 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, BUNO22a, BBC^{+21b}, BOPJ^{+21b}, CX21a, CGSP24b, ETT21a, GPM21a, GKA^{+23a}, HAC^{+23a}, KE23a, KFTB20a, KSS21a, KWMPR24a, KK22b, MLG^{+21a}, QLW^{+22a}, RPD^{+20b}, SWM^{+20a}, dRHB21, SNK24a, SSFS22a, TTH^{+21b}, TCS^{+21b}, VV20a, WTST24b, WLSC23b]. **coverages** [VHS⁺²⁴]. **COVID** [SLMA21].
COVID-19 [SLMA21]. **Cp** [HSG21, WLZM20]. **CR** [WLZM20, MYYS24, Wan23, XDZ23]. **Cr-doped** [XDZ23]. **create** [ZK23].
created [ARR22a]. **creating** [LKM20]. **Criegee** [SK20]. **Critical** [SB20, dSCCN21, MT20b]. **CrMnSi** [WZW⁺²⁴]. **cross** [ABZ20b, ALA20, CV22, KGTL21, ZK23, dBCdL20]. **cross-coupling** [ABZ20b]. **cross-link-assisted** [KGTL21]. **cross-platform** [ZK23].
cross-sections [CV22, dBCdL20]. **crossing** [SaATR24, WTST24a]. **crucial** [KE23b, MBBU23]. **cryo** [LSP23, PJJL23, Yos24]. **cryo-electron** [Yos24].
cryo-EM [LSP23, PJJL23]. **Crystal** [GLC⁺²², SGSB23, AK20, CX23, KZP22, MZ21, RDS⁺²⁰]. **crystallin** [FLT23]. **Crystalline** [HZG⁺²⁰, Cer22, PDGD22]. **crystals** [BEKM24, LT23, LWF⁺²², NMF121]. **Cs** [SL20, AQIS⁺²⁴, BEKM24].
CSiGaAl [DC22a]. **CsPbBr** [BBL⁺²²]. **Cu** [MH20, AD20, JGSA22, LZW⁺²³, PP23, SPSH20]. **cube** [Ba20b]. **cupric** [XZZ⁺²⁰]. **Current** [BSL20, SPT21, SZL23]. **Current-Flow** [BSL20].
Curvature [MA23a, PRIP24]. **Curvature-weighted** [MA23a]. **cut** [WKL22]. **cut-offs** [WKL22]. **cutoff** [DO20]. **cyanomethylation** [DSK21].
cycle [Dor20, MKB⁺²¹]. **cyclin** [TWT⁺²²]. **cyclin-dependent** [TWT⁺²²].
cyclization [TYZ20]. **Cycloaddition** [LSC24, BAM⁺²⁴, KZJ22, MGCM21, NMMC21, SVTK⁺²², SMB⁺²³].

cycloadditions [SVR⁺24, SHH⁺24]. **cyclobutanes** [HCY⁺22].
cyclocondensation [MIP⁺22]. **cyclodextrin** [IAS⁺24]. **cyclohexaborate**
 [JWS⁺24]. **cyclooctatetraene** [KK22c]. **cyclopenta** [MSE⁺21].
cyclophosphamide [DSS⁺24]. **cyclopropane** [SM23, WG20].
cyclotrimerization [ZMH⁺21]. **cysteine** [dMBdAVdS24, dSCCN21].
cytosine [LRqG⁺22].

D [BBY⁺21, DF22, FLT23, GSJ⁺23, Mon24, Pan23, PSM⁺20, SS20, TPZ⁺20,
 TZS⁺22, WKL22, dCVARN20]. **D-crystallin** [FLT23]. **D3**
 [FBM⁺23, RMJ21]. **D4** [NG20]. **D614G** [ONA⁺20]. **damaged**
 [CGMRVBAl22, LRqG⁺22]. **darunavir** [CBK⁺24]. **Data** [BK22, ENR⁺24,
 SK20, TV22, XZ20, BMT⁺21, GG22, IMT⁺21, LL22, RD24, SWLC22].
Data-driven [TV22]. **database** [AZKM22, CBB⁺21, LRKD23, GLC⁺22].
databases [LGD⁺20, ZK23]. **datasets** [KZOV23, VT24]. **Dative**
 [PTP23, YSMS24]. **daunting** [DRBT24]. **DD** [CD20]. **DD-peptidase**
 [CD20]. **deacylation** [CD20]. **deal** [DWSX20]. **Deciphering** [HD21].
decker [AS23]. **Decoding** [MIP⁺22, OTZW24]. **decomposed** [NVBG23].
decomposition [AV20, AK20, CL23, HUUO23, JCMHT22, LHG⁺23,
 MSA⁺24, MGCM21, MT20b, OTZW24, SSM21, TSZ⁺21, YMM⁺24, ZG21].
decomposition-based [MT20b]. **decoration** [SDK20]. **decreasing**
 [HD21]. **dedicated** [CBB⁺21]. **Deep**
 [LPP20, PMT⁺22, JGK⁺22, MLP22, WLSC23a]. **deeper** [DGM22]. **deeply**
 [PDGD23]. **DEER** [QLC⁺20]. **defective** [PSM⁺20, SPT21]. **defects**
 [CTBB20, GPEK⁺20, PGP⁺21, PKT21]. **Deformation**
 [FMFG20, NVBG23, PGDD24, RA20]. **degenerate** [NSKN21]. **degrees**
 [DB23]. **dehydration** [KSS21b, KSRB⁺21]. **dehydrogenated** [ONC20].
delayed [LYX⁺22]. **delivers** [ZWY⁺22]. **delivery** [AAID22].
delocalization [LKAT22, RTB23]. **delocalized** [BdLC21, MG24]. **delta**
 [HNCL24]. **Densities** [WG21, Pil20, SZL23, TAC⁺23, Wan21a, Wan21b].
Density [BBK20, CFOMCB⁺22, CWZD20, CMD⁺22, FMFG20, KZJ22,
 MLB⁺23, RMJ21, RA20, SK20, TANC23, YXGZ20, APS20, AS21,
 ABAQ⁺23, BWS20, BA22, Ben22, BSF20, BBK⁺21, BOPJ⁺21a, CHVF21,
 CPG21, Cer22, CQSG20, ĆPP⁺22, CTBB20, DRBT24, DZL⁺20, DOT22,
 EPT21, FB20, GH22a, GD23, GAP21, HTTT23, HM21, HGR⁺24, HCS⁺20,
 HLV⁺24, IYI⁺20, IW24, KZJ21, KS21, KdILC22, LRF⁺21, LSC24, MWK⁺20,
 MNH21, MH22, MKK⁺22, MAM21, MFS22, MKB⁺21, MGCM21, MH20,
 MSE⁺21, MBBU23, MSS20, NG20, NSH23, NEG⁺20, NVBG23, NN20,
 OTZW24, OE20, OMC⁺20, OAN⁺23, PCB⁺24, PDP⁺24, RCC⁺20, RC22,
 RTB23, SDK20, SWF⁺20, dASRHB21, SC22, SMB⁺23, SSYB⁺20, SZP⁺20,
 TLS23, TT20, VV20b, WKCP21, XSP⁺23, ZHHS21, ZZ23a, dBCdL20].
density-based [HTTT23, HGR⁺24]. **density-fitted** [BSF20].
density-fitting [HGR⁺24]. **Density-functional**
 [TANC23, BWS20, NEG⁺20]. **density-matrix** [IW24]. **Depend**
 [BWM20, BA24]. **Dependence** [JK21, YXGZ20, MH20, SBD⁺21].

dependencies [BK22]. **Dependent** [YXGZ20, BA22, CPG21, FB20, FNY21, IYI⁺20, IN23a, JRS20, MFS22, MSS20, Nan24, Ngo21, OMC⁺20, OAN⁺23, SZL23, TWT⁺22, TANC23, XZW⁺21, XAD20]. **deposited** [VTdlM20]. **deposition** [MSA22a]. **Derivation** [FMFG20]. **derivative** [CC22]. **Derivatives** [GRN20, BHR⁺21, CFOMCB⁺22, CMO⁺24, CCPR24, JAP⁺24, KLC⁺24, KK22c, SEBE21, SGGG22, DMTR22, SM23, TANC23, ZWL24b]. **Dermocybin** [RPA⁺24]. **describe** [GAP21, IK21]. **described** [KKAK23]. **Describing** [HPM⁺21, MH22, RLHG⁺23]. **Description** [BLP20, HRT⁺20, XCJ20, ZLLL22]. **descriptor** [CMO⁺24]. **descriptors** [BHR⁺21, CMD⁺22, COK22, GJMPVR⁺20, HBT⁺20, LGM20, LGM22, NTK21, PDP⁺24, TCS⁺21a, YGG⁺23]. **Design** [IW23, PAS⁺20, SEBE21, BXY⁺24, BBB⁺23, CBK⁺24, DSK21, GLC⁺22, HKFT21, KI24, LSP23, LYX⁺22, LHH⁺23, NPGP23, PMT⁺22, PSB⁺22, RKC21, RDK⁺22, SHP⁺23, YYZ⁺21, ZZG⁺21, ZBH⁺23]. **designs** [YBS⁺20]. **desirable** [NPGP23]. **detailed** [NP23, SY21]. **details** [TYZ20]. **detection** [CR24]. **determinant** [BTSB22]. **Determination** [NNT⁺20, CST23, FKT21, LHB⁺24]. **determines** [HYA⁺20]. **Determining** [WZZ⁺20, KPHV23, SFS24, VHS⁺24]. **deterministic** [TS21]. **Developing** [HKFT21]. **Development** [AFR⁺24a, BTL24, IL24, KG23, KTBS23, LRqG⁺22, SKL23, SHH⁺23b, SHH⁺23a, WSL⁺20, GKO⁺22]. **developments** [VWFR21]. **devices** [AMF⁺20, LAM⁺23, SPT21]. **DFT** [TANC23, AK20, AS23, ABNG22, BSR22, CS20, Cha24, CL23, DK23, DSK21, FCB23, FBM⁺23, FV20, HS22, JAP⁺24, JMV21, KMR⁺24, KLC⁺24, KKAK23, LCC⁺21, LT23, LLJ⁺24, LDT⁺22, MPOC21, MJS⁺23, MCD22, MK22b, NG20, PLT24, RLHG⁺23, SVDS21, dSSCC24, SB20, SLML24, TANC23, TAB⁺24, TMO⁺21, WD20, WS21, WKG⁺23, YC23, ZRSST20, ZDBZ20]. **DFT-based** [dSSCC24]. **DFT-D4** [NG20]. **DFT/MRCI** [ZRSST20]. **Di-** [KZP22]. **diagnostic** [SD21]. **diagonalization** [BMT23, MB21, WFLZ23]. **diagonalization-free** [MB21]. **diagrammatic** [HD21]. **diagrams** [PDC23, SGSB23, VFCG20]. **dianionic** [DPSG20]. **diaqua** [MVP⁺20]. **diatomic** [AA20, Tze21]. **diatomics** [KW22]. **diazadiboretidine** [NHFS21]. **diborane** [SLML24]. **dicarboranyl** [PGP⁺23]. **dications** [SMH21]. **dichalcogenide** [PSM⁺20]. **dichroism** [MSA22b]. **dichromium** [MVP⁺20]. **dicopper** [MVP⁺20]. **dielectric** [MLM⁺24, RMS⁺23]. **Diels** [MNZGO⁺20, MGCM21, NMMC21, SSYB⁺20]. **diene** [NMMC21]. **dienes** [BXY⁺24]. **differences** [WFBB22]. **different** [JGdC⁺23, DO20, DWSX20, KK23, Sts20, WS21]. **differential** [SD21]. **differently** [AST24]. **diffuse** [MCP23]. **diffusion** [BUNO22b, CGMRVBAl22, FNY21, PFSC20, RGGD21, SM22b, UKBD23]. **diffusion-controlled** [CGMRVBAl22]. **diffusivity** [NS22]. **difluoro** [SKGG23]. **difluorocarbene** [ZS22]. **difluoromethane** [BR23]. **digestion** [Nee23]. **dihalogens** [RZS⁺23]. **dihedral** [RR22]. **Diimides** [NRH⁺20]. **diimine** [WCD⁺23]. **diketones** [AV20]. **diketopyrrolopyrrole** [dCB23]. **dimensional**

[GVJ⁺22, KGS⁺21, LWLC21, PPV⁺21, dSSCC24, STB⁺20, Yos24, YAO20].
dimer [BCN22, JC20, Kop22a, SAZ⁺23, YrYqLhC23]. **Dimerization**
 [WGKG20, BVC⁺23]. **dimers** [BD22, MC23, WCD⁺23]. **dimethylfulvene**
 [SHH⁺24]. **dinickel** [LLKS23]. **dinitrate** [GJL21]. **dinitrogen**
 [Ano24a, DGM22, KJV23, SK23, ZYZ24]. **diol** [BBBP⁺23]. **diols** [MLGY24].
dioxaphosphole [MSE⁺21]. **dioxaphosphole-2-sulfide** [MSE⁺21].
Dioxide [SB20, BR23, ZSD⁺20]. **Dipolar** [SVTK⁺22]. **dipole**
 [BS23, BSF20, HPG20, LRKD23]. **dipole-coupled** [BS23]. **Direct**
 [FMFG20, KM24, YW20]. **Directing** [AD20]. **directions**
 [BBSFA22, MAM21, YAO20]. **Discovering** [CGSP24a]. **Discovery**
 [WZW⁺24, CDCT21, CBK⁺24, LHH⁺23, MNBG⁺21]. **Discriminating**
 [CX23]. **Disentanglement** [CB20]. **Dismantlement** [YOCMA23]. **disorder**
 [DB23]. **disordered** [SY21]. **disparity** [DWSX20]. **dispersion**
 [CTBB20, MBBU23, RMJ21]. **dispersion-corrected** [CTBB20].
displacement [Ano24a, CB20, SK23]. **displacements** [MAM21].
disruption [MDO⁺20]. **dissimilar** [MPP23]. **Dissociation**
 [DHN⁺21, DK23, MPP23, SNW22]. **Distance**
 [LLS22a, KPR23, QLC⁺20, SKKG22]. **distinct** [NS22]. **distortion**
 [ETT21b, PDL24]. **Distributed** [GJMPVR⁺20, LRKD23]. **distribution**
 [IN23b, Ore24, QLC⁺20, Tou21]. **distributions**
 [LBH⁺22, MVV22, SKKK20]. **disubstituted** [SaATR24]. **disulfanediylbis**
 [MSE⁺21]. **Divalent** [PAS⁺20, ALA⁺22]. **diverse** [BUNO22b, KS21].
Divide [JGM21, FKT21, NN20, SY21]. **divide-and-conquer**
 [FKT21, NN20, SY21]. **DJMol** [PSGL21]. **DLPNO**
 [CS20, CK22, Dor20, GRBN21, MCP23, PRF20, Sán20, SI22].
DLPNO-CCSD [CS20, CK22, Dor20, MCP23, PRF20, SI22].
DLPNO-CEPA [Sán20]. **DLPNO-CEPA/1** [Sán20]. **DMRG** [LJW⁺23].
DMRG-CASSCF [LJW⁺23]. **DNA**
 [BVGB23, FVSS20, FBP⁺22, HKS20, SBFSJMLU23, SGGG22]. **DNN**
 [XLW⁺22]. **do** [CPG21, GUCCR20, ZGZC20]. **Dock**
 [Min20, AG21, BTC24, PSB⁺22]. **Docking**
 [XZ20, BTC24, BAO⁺20, CFOMCB⁺22, LYKS23, MZMK⁺21, MSA22a,
 PPP21, RKC21, TZS⁺22, VWP⁺22, YC23]. **dodecahedrane** [JC20].
dodecyl [ZK21]. **Does** [BA24]. **DOI** [MT20a]. **Domain**
 [PT20, PW20, TLD⁺22, BVC⁺23, GRBN21, San21]. **Domain-based**
 [PW20]. **donation** [GAG20]. **donor** [JGdC⁺23, DDSM23, PTP23].
donor-pyrene [JGdC⁺23]. **dopamine** [TPZ⁺20, TZS⁺22]. **doped**
 [DZL⁺20, DOT22, WMJ⁺22, XDZ23, ZDBZ20, ZWL⁺24a]. **dot** [LCLB24].
Double
 [FV20, OMC⁺20, AQRA⁺23, AQMM⁺23, BOPJ⁺21a, CPG21, RMBSPJSG24].
double-hybrid [BOPJ⁺21a, RMBSPJSG24]. **Doubles** [HFPS20].
downregulation [CSP20]. **downward** [ETT21b]. **DPC** [ZK21]. **DPP**
 [dCB23]. **drive** [RLR⁺20]. **driven**
 [AIV20, AR24, MP24, SBFSJMLU23, San21, SSS⁺20b, TV22, YJZ⁺22].

Drude [BS23, KLP⁺²², KYM20, LJ20, ODL20]. **Drug** [SLMA21, AAID22, CBK⁺²⁴, DYGM21, HKFT21, LSP23, RKC21, RDK⁺²², SSPK24]. **drug-delivery** [AAID22]. **drug-like** [DYGM21]. **druglike** [SHH^{+23b}]. **drugs** [HS22, HS23, HBM⁺²⁰, KMR⁺²⁴, NST⁺²⁰, PRH20, dCRM21]. **Dual** [YW20, MPP23]. **dual-atom** [DLH⁺²³]. **Dual-hybrid** [YW20]. **due** [FBP⁺²², MAM21, ÖLP⁺²⁰, SSPK24]. **dyes** [TMO⁺²¹]. **dynamic** [BAO⁺²⁰, BBBP⁺²³, IAS⁺²⁴, MPOC21, MK22a, PCB⁺²⁴, SYS⁺²¹]. **dynamical** [RR22, SZL23]. **dynamically** [MT20b, TWT⁺²²]. **Dynamics** [FMFG20, HHL⁺²⁰, KUNT20, YXGZ20, Zac20, AiIS⁺²¹, ALA⁺²², BUNO22b, BAO⁺²⁰, BR23, BTL24, BBL⁺²², CDCT21, CSP20, CST23, CCPR24, DHN⁺²¹, FMK24, FNY21, FBP⁺²², GGK20, GK24, GG22, JRS20, JKK⁺²¹, KR23, KOD21, KLP⁺²², LL21a, LKM20, LHH⁺²¹, LEP⁺²¹, MN20, MKK⁺²², MGB⁺²², MSA22a, MAP⁺²⁰, NLC23, Nan24, NN20, NP23, OSHT20, PBM21, PDL⁺²¹, POvG21, PGP⁺²³, PPP21, PM21, QLC⁺²⁰, RKC21, RDK⁺²², RGGD21, RPD^{+20a}, SPSH20, Shi22, SY21, SWLC22, SCC⁺²², SSPK24, SSFS22b, SKKK20, SCCZ21, TPB22, UKBD23, VCRP23, WTST24a, WSV20, WCT⁺²³, WFBB22, WKD⁺²¹, YC23, YMM⁺²⁴, ZG21, ZWY⁺²², ZFRM20].

E-fields [AMF⁺²⁰]. **E4** [WS21]. **earth** [ZWL^{+24a}]. **earth-doped** [ZWL^{+24a}]. **ebsele**n [YC23]. **EDA** [DGM22, GM22, GKA^{+23b}, SM23]. **EDA-NOCV** [DGM22, GM22, GKA^{+23b}, SM23]. **edge** [CS23]. **Effect** [AD20, DLH⁺²³, GRN20, JC20, ARR22a, BMA⁺²⁴, CBF⁺²⁰, DO20, FMK24, FVSS20, JMK⁺²⁰, KPHV23, KEK23, LK22, LLZ⁺²³, MAM21, MEKH22, dCB23, PRH20, SaATR24, Sts20, SCZ⁺²¹, XZW⁺²¹]. **effective** [BBC^{+21a}, KKAK23, UB20]. **Effects** [DK23, JFZ⁺²⁰, KPDB22, KTM⁺²³, MSA22a, SLR⁺²⁰, SGT⁺²⁰, JGdC⁺²³, BAM⁺²⁴, CMG⁺²⁴, CMO⁺²⁴, CX21b, FBP⁺²², GCP22, GAG20, KWYN23, LCLB24, dCB23, MCD22, PCI23, SSSA23, WCY⁺²⁴, dCVARN20]. **efficiency** [FYIO23, ZWL24b]. **Efficient** [CSGVF⁺²⁰, LMPT21, MN20, MR21, MKB⁺²¹, MT20b, PPV⁺²¹, RCC21, XLW⁺²², AD23, DYGM21, EK20a, KG23, KSRKS21, RD24, TAB⁺²⁴, ZQ24, ZZG⁺²¹]. **efflux** [CGSP24a]. **effort** [POvG21]. **eigenvalues** [KDLP21]. **Eighth** [PSMPB21]. **Eighth-Shell** [PSMPB21]. **elacestrant** [CSP20]. **elastic** [KOD21, LM24, MA23a, MA23b, MMAZ⁺²³, ZLLL22]. **Electric** [PL22, SHM⁺²⁰, ZG21]. **electride** [Ari24, DSC20]. **electrocatalysts** [AR20]. **electrochemical** [KDLP21, KF24]. **Electrocyclization** [PC21]. **electrode** [DOT22]. **electrolyte** [LEP⁺²¹]. **electrolytes** [EG20, HM21]. **Electron** [KZJ22, BJ22, BBC^{+21a}, ČNF23, EVKL21, EPT21, IN23a, KZJ21, LKT21, LKAT22, LT23, MH22, MAM21, PTP23, PDP⁺²⁴, RCC⁺²⁰, RNP20, RTB23, SS20, SPSH20, SMB⁺²³, SSO⁺²⁰, SZL23, TAC⁺²³, Yos24, ZYZ24, dBCdL20]. **electronegativity** [Vyb23]. **Electronic** [DGSB⁺²⁰, JX24, SBFSJMLU23, SM22b, SCKH21, TT20, AQIS⁺²⁴, ABAQ⁺²³, Ari24, AMF⁺²⁰, BMA⁺²⁴, BTSB22, CC22, CCPR24, HSG21, IK21, JMV21, KWYN23, KPDB22, Kop22a, LM24, LXP⁺²², LAM⁺²³,

MNH21, MML⁺²³, MNZGO⁺²⁰, MSA22b, MP23, NHFS21, OSHT20, PSM⁺²⁰, RvWH23, RCC⁺²⁰, SS24, SGT⁺²⁰, STB⁺²⁰, TPZ⁺²⁰, TSH⁺²³, UR23, VM23, WMJ⁺²², XZW⁺²¹, XDZ23]. **electrons** [MP23, PDGD23]. **electrooxidation** [DOT22]. **electrophilicities** [HBT⁺²⁰]. **Electrophilicity** [PC23]. **electrostatic** [AS20, HS23, JGGPN21, KS24, LWLC21, LDT⁺²², MMK⁺²⁰, ÖLP⁺²⁰, UB20, VL22, ZZ23a]. **Electrostatically** [TSR21]. **Electrostatics** [HRT⁺²⁰, BSB⁺²⁴, SCvW22, YFH⁺²¹]. **element** [BSB⁺²⁴, PLZT23]. **elementary** [DGSB⁺²⁰, SYS⁺²¹]. **Elementometalation** [WLZM20]. **elements** [GPM21b, Klo22, NUK21, RCC21, RNP20]. **elimination** [KZJ21]. **Elongation** [MMK⁺²⁰]. **Elucidating** [NST⁺²⁰]. **Elucidation** [SKGG23, HRTSS⁺²⁰]. **elusive** [DDSM23]. **embedded** [BVGB23, LLJ⁺²⁴, TSR21]. **embedding** [DGSB⁺²⁰, IRB⁺²³, LWLC21, LDT⁺²², MMK⁺²⁰, UB20]. **embrittlement** [ZFRM20]. **emission** [AS20, FB20, KBK⁺²⁴]. **emitters** [LYX⁺²²]. **Emodin** [RPA⁺²⁴]. **Empirical** [LJ20, KB22, PWX⁺²⁰, PNT⁺²², RLHG⁺²³]. **employing** [MAI22]. **enable** [BTC24]. **enabled** [BCN22, LBH⁺²²]. **Enabling** [ENR⁺²⁴]. **Enantiomerization** [LLJ⁺²⁴]. **enantiomers** [IAS⁺²⁴]. **enantioselective** [IAS⁺²⁴]. **enantioselectivities** [BXY⁺²⁴]. **Encapsulation** [CBF⁺²⁰, DSC20, SSSA23]. **Encoding** [GJMPB⁺²⁰]. **End** [MXM20, Ano24a, SK23, TANC23, TTK23]. **end-group** [TANC23]. **end-on** [Ano24a, SK23]. **End-Point** [MXM20, TTK23]. **ended** [GSD⁺²²]. **ending** [SVR⁺²⁴]. **Endo** [Jab22a]. **Endo-** [Jab22a]. **endohedral** [DA22, LXP⁺²²]. **endpoint** [SHH^{+23b}, SHH^{+23a}]. **ene** [SMB⁺²³]. **energetic** [JMV21, LWC⁺²⁴, PYA24]. **energetically** [NSKN21]. **Energetics** [HHL⁺²⁰, NG20, NDK24, PM21, WGKG20]. **Energies** [BBK20, FMFG20, HFPS20, MFC20, NRH⁺²⁰, AD23, BBY⁺²¹, BOPJ^{+21a}, BCN22, FCB23, Fed22, GZFSM21, HCS⁺²⁰, KRW⁺²⁴, KPHV23, LCC⁺²¹, MPP23, MLB⁺²³, MEKH22, MCP23, NTK21, ÖLP⁺²⁰, OM22, PRF20, PFSC20, PGH24, TTK23, TTT⁺²¹, VV21]. **Energy** [FKT21, GRN20, KPR23, LPP20, MXM20, Min20, NNT⁺²⁰, SZLD20, YYS20, APP24, AV20, ARR22a, AKGD24, AQRA⁺²³, AK20, AA20, BBC20, BJ22, BBC^{+21a}, BF22, CC22, CSGVF⁺²⁰, CdSB⁺²¹, CSWW20, CSP20, DC22a, ERVN24, GH22a, GBM20, GVJ⁺²², HB21, HBM⁺²⁰, HNCL24, HPM⁺²¹, JK21, JCMHT22, JGM21, KG23, KK23, KFTB20b, Kop22b, Kos22, LM24, LPF⁺²³, LWF⁺²², LML⁺²³, LHG⁺²³, MML⁺²³, MN20, MSL⁺²⁰, MSA⁺²⁴, MGCM21, MBBU23, NUK21, NTK21, NMFI21, NI22, NML21, OTZW24, OKI⁺²¹, PPV⁺²¹, PDC23, PCB⁺²⁴, RDB23, RH21, Sán20, SSS^{+20a}, SY21, SDH23, Sts20, SCCZ21, SHH^{+23b}, SHH^{+23a}, TWT⁺²², TSZ⁺²¹, THH⁺²⁴, TM20, TAB⁺²⁴, TSH⁺²³, VL22, Vyb23, WTST24a, WCT⁺²³, WFBB22, WdGG24, XLW⁺²², XZC⁺²⁴, YBS⁺²⁰, YFH⁺²¹, ZQ24, ZK21]. **energy-adjusted** [GH22a]. **Energy-based** [FKT21, LWF⁺²²]. **energy-efficient** [TAB⁺²⁴]. **energy-related** [CdSB⁺²¹]. **enforced** [WCD⁺²³]. **engineering** [SZP⁺²⁰]. **enhance** [YYZ⁺²¹]. **Enhanced**

[FMFG20, OC23, WLSC23a, BPT⁺23, DWSX20, KLZ⁺23, LGC21, MH20, MMAZ⁺23, ONA⁺20]. **Enhancement** [MSA⁺24]. **enol** [LKAT22]. **enrichments** [KDP⁺22]. **ensemble** [HTFY21, HBM⁺20, QLC⁺20, RD23, WYC⁺24, XLW⁺22]. **ensembles** [NML21]. **entangled** [WKD⁺21]. **entanglement** [dSSCC24]. **entatic** [RLHG⁺23]. **enter** [APS20]. **enthalpies** [Dor20]. **entirely** [BdLC21]. **entropy** [YJZ⁺22]. **entropy-driven** [YJZ⁺22]. **entry** [GG22]. **ENUF** [YLZ⁺20]. **Enumeration** [SZLD20]. **environment** [BBB⁺23, KCF⁺20, NUK21]. **enynes** [HCY⁺22]. **Enzymatic** [SHM⁺20, PRF20]. **enzyme** [AR24, DPSG20]. **ePharmer** [MLG⁺21b]. **epidermal** [BHR⁺21]. **EPISOL** [CKH23]. **epoxides** [WKG⁺23]. **equalization** [Vyb23]. **equation** [BSB⁺24, NSRK21, Nan24, RCC21, SCvW22]. **equations** [MB21, MT20b]. **equatorial** [SVDS21]. **equilibria** [CM20a, CA22]. **Equilibrium** [dSCCN21, KS21, MMF⁺24, SFS24]. **equivalent** [KF24]. **Erratum** [MT20a]. **error** [KM22, UKBD23]. **ESCASA** [LL21b]. **Escherichia** [CGSP24a]. **ESES** [UYJ⁺24]. **essential** [GLC⁺22]. **establish** [RCC⁺20]. **Establishing** [LWC⁺24]. **estimate** [LRKD23]. **estimates** [AD23, CR24]. **Estimating** [LBH⁺22, Ngo21, BK22]. **estimation** [AKGD24, JGM21, KZP22, KG23, LL21b, TTK23]. **Estimations** [TTT⁺21]. **estimator** [AZKM22, Vyb23]. **estrogen** [CSP20]. **ethane** [MLX⁺24]. **ethanol** [KGS⁺22]. **ethenediol** [MLGY24]. **ethyl** [MIP⁺22]. **ethylene** [HCY⁺22, MYYS24, MCD22, PLZT23, SVTK⁺22, SJZ⁺21]. **ethylenediamine** [MIP⁺22]. **ethylhexanoate** [BR23]. **ETS** [SBB⁺22]. **ETS-NOCV-based** [SBB⁺22]. **Eu** [ALA⁺22]. **Eulerian** [UYJ⁺24]. **europium** [HRTSS⁺20]. **Evaluating** [dSSCC24, TZS⁺22]. **Evaluation** [BHR⁺21, KS21, MZMK⁺21, MCD22, PRH20, VAL20, BBB⁺23, DWZ22, Gao20, LLZ⁺23, MLB⁺23, SEBE21, SSS⁺20a, ZZ23a, SHH⁺23a]. **even** [RD24]. **events** [RLR⁺20, RD23, VZG⁺24, WRBT21]. **evidence** [CNF23]. **Evolution** [GJL21, MM20, CG20, CCPR24, DLH⁺23, KdLc22, MIP⁺22, PSB⁺22, WMJ⁺22, YYS20]. **Evolutionary** [CH23]. **Ewald** [Pan23, YLZ⁺20]. **Examining** [NGD22]. **Exchange** [BBK20, MBBU23, AA20, HM21, JKS23, KN21, KK23, KKAK23, LKT21, MH22, MGB⁺22, MZMK⁺21, MM24, RMJ21, RR22, SEZ20, TV22, VV20b, XZX⁺22, YW20]. **exchange-** [MM24]. **exchange-correlation** [AA20, HM21, MH22]. **excision** [LRqG⁺22]. **Excitation** [HFPS20, HCS⁺20, NRH⁺20, FCB23, Kos22]. **excitations** [BOPJ⁺21a]. **Excited** [AIV20, Tou21, VM23, AST24, Ari24, BGPR24, BMT23, CG20, CPG21, FCB23, FB21, FMK24, Gie21, HD21, HPM⁺21, IK21, JCMHT22, KL20, KWB24, LHH⁺21, OSHT20, OMC⁺20, OAN⁺23, RDS⁺20, Sts20, WD20, WFLZ23, ZRSST20]. **Excited-state** [AIV20, WD20, ZRSST20]. **excitonic** [SBD⁺21]. **Exhaustive** [BAO⁺20, SZLD20]. **exhibited** [Wan23]. **exhibiting** [LYX⁺22]. **existence** [OAC23]. **exohedral** [Jab22a]. **expanded** [CKH23, NML21]. **experiment** [THH⁺24]. **experimental** [AZKM22, BMT⁺21, GG22, HBT⁺20, HLV⁺24].

experiments [Yos24]. **Explainable** [KI24]. **Explicit** [MGB⁺22, CCHS23, LKT21, PGH24, RPD⁺20a, WLSC23a].
explicit-implicit [RPD⁺20a]. **explicitly** [LRKD23, SM22a]. **Exploration** [GVJ⁺22, OY20, RKC21, LGJF22, LLKS23, OC23, OKI⁺21, RSHG23, SDK20, San21]. **Explorer** [SSFS22b]. **Exploring** [AVM21, MSL⁺20, NTK21, SGRN24, SCCZ21, THH⁺24, YC23]. **expressed** [HCS⁺20]. **expression** [UKBD23]. **Extended** [GX20, RGD21, BPT⁺23, DWSX20, KGD⁺21, NBE⁺23, PSMPB21, KWX23]. **Extending** [PGH24].
Extension [AYO20, JCMHT22]. **External** [GD23, BW22b]. **extraction** [ENR⁺24]. **extrapolation** [SCKH21]. **extremely** [JKK⁺21, RBM⁺23].

F [APR21, SCC⁺22, Ben22, GGK20, MPV22]. **F-NMR** [Ben22]. **F12** [CK22, DKB23]. **facilitate** [SIW21]. **Facilitates** [VDK⁺20]. **Facilitating** [Zac20]. **facilitator** [QLC⁺20]. **Factor** [KM22, BHR⁺21, CC22, GKA⁺23b, SCCZ21]. **Factors** [AD20, Cha24, DPY⁺22, XZX⁺22]. **fail** [JRS20]. **fail-safe** [JRS20]. **fair** [DGM22]. **FAIRness** [RTB⁺22]. **FALDI** [BdLC21]. **families** [FB21]. **Fanpy** [KRSD⁺23]. **Fast** [MPR22, VV21, YAO20, AYO20, AiS⁺21, CRT⁺21, JCMHT22, MY24, MLX⁺24, MSS20, NML21, RB22, TSZ⁺21, YLZ⁺20, ZZ23a]. **fate** [CSG⁺21].
FCclasses3 [CS23]. **FCI** [dSSRVdM24]. **Fe** [HSG21, IK21, LXP⁺22, SM22b, MYYS24, ZFRM20]. **Fe-C** [ZFRM20].
Features [SHM⁺20]. **featuring** [ZMH⁺21]. **FeO** [HUUO23]. **FePS** [EK20b].
FePSe [EK20c]. **Fermi** [ASW20]. **ferrimagnets** [WZW⁺24]. **ferrocenium** [CS20]. **Feshbach** [BBY⁺21]. **FFLUX** [HRT⁺20, KSP21, MP24]. **FFParam** [KYM20]. **FGFR3** [MKSS20]. **FH** [TTT⁺21]. **Field** [BAC20, LJ20, WSL⁺20, ALA⁺22, BJ22, BTL24, CV22, CTPJH22, FVSS20, GKO⁺22, IW24, KLP⁺22, KYM20, LRqG⁺22, MT21, MAKZ23, ODL20, PLP⁺20, PL22, SPSH20, TPB22, VHS⁺24, WLWR22, WKD⁺21, YFH⁺21, ZG21, ZWY⁺22]. **field-based** [MAKZ23]. **field/vibrational** [CV22]. **Fields** [SHM⁺20, AMF⁺20, DHD21, GD23]. **Fields-Features** [SHM⁺20]. **fifth** [LB22]. **file** [VAP⁺21]. **files** [PBM21, VAP⁺21]. **finding** [RSHG23]. **fine** [XZC⁺24]. **fingerprinting** [KI24]. **fingerprints** [SKL23]. **finite** [BSB⁺24].
First [DBE20, EPT21, KDKS21, LM24, AWK⁺23, BRNB21, DLH⁺23, EK20b, KPKS23, PM21, SS24]. **First-Principles** [DBE20, KDKS21, DLH⁺23, EK20b]. **fission** [LCP21, SCKH21]. **fitness** [ONA⁺20]. **fitted** [BSF20]. **Fitting** [ALA20, BK22, BK24, CQSG20, HGR⁺24, MFS22, MSS20, NSH23, TAC⁺23, ZZ23a]. **Five** [AD20, HGF20, LLJ⁺24, PLP⁺20]. **Five-Coordinate** [AD20].
five-membered-heterocycle-embedded [LLJ⁺24]. **five-site** [PLP⁺20].
fixation [JAP⁺24]. **fixed** [PLP⁺20]. **fixed-charge** [PLP⁺20]. **fixing** [DGSB⁺20]. **flavins** [CA22]. **flexibility** [BBSFA22, SPSH20]. **Flexible** [HRT⁺20, Min20, VWP⁺22]. **flip** [IYI⁺20, KKAK23]. **Flow** [BSL20, AFR⁺24a]. **fluctuation** [SH23, XZW⁺21]. **fluid** [CM20a]. **fluids**

[SSYB⁺20]. **fluorescence** [AS21, LYX⁺22]. **fluorescent** [BVGB23, ZRSST20]. **Fluorine** [OE20]. **fuoro** [BAM⁺24]. **fluorophores** [FMK24]. **flupyradifurone** [BTL24]. **flux** [MNZGO⁺20]. **fly** [APP24, OSHT20, RBM⁺23]. **focal** [BSF20]. **focal-point** [BSF20]. **Fock** [BTSB22, BBK20, NSH23, NI22]. **Fold** [CLS⁺20]. **Folding** [GG22, CH23, SSS⁺20b]. **Foldy** [IWN24]. **Following** [CG20, KdILC22, ETT21b]. **Force** [BAC20, LJ20, QB20, WSL⁺20, ALA⁺22, BJ22, BTL24, DHD21, FVSS20, GKO⁺22, KLP⁺22, KYM20, LRqG⁺22, MT21, MNZGO⁺20, MAKZ23, ODL20, PPV⁺21, PLP⁺20, TPB22, WLWR22, YFH⁺21, ZWY⁺22]. **force-field** [GKO⁺22]. **forces** [BW22b, KRW⁺24, KSP21, LCC⁺21]. **Form** [CWZD20]. **formally** [SSP23]. **formamide** [NHFS21]. **Formation** [GOY20, LZW⁺23, HL20, KPDB22, MDO⁺20, MLM⁺24, SSS⁺20a, dSSRVdM24, SKGG23, ZZ23b]. **formats** [VAP⁺21]. **formed** [SKT24]. **formic** [FP23]. **forms** [DSC20]. **formula** [Pan23]. **formulas** [IN23a]. **formulation** [CK22, Fed24]. **formulations** [SCvW22]. **foundation** [TSH⁺23]. **Four** [Yos24, DSB23, KWYN23]. **four-component** [KWYN23]. **Four-dimensional** [Yos24]. **four-membered** [DSB23]. **Fourier** [YLZ⁺20]. **Fractional** [ASW20]. **fracture** [MMAZ⁺23]. **Fragment** [CLS⁺20, KUNT20, AKN⁺20, BSS⁺22, BBC⁺21a, Fed22, Fed24, MSA⁺24, NUK21, NAN⁺23, TWT⁺22, UB20, ZK23]. **fragment-based** [UB20]. **Fragment-Free** [CLS⁺20]. **Fragmentation** [AKN⁺20, SD21, LWF⁺22, VWJ23]. **FRAGMENTISE** [ZK23]. **Fragments** [AD23, LML⁺23, PTP23, RTB23, SSP23]. **Fragments-in-fragments** [AD23]. **Framework** [GRN20, LPP20, CM20a, GUCCR20, HRTSS⁺20, KZJ21, WMZJ20, WFBB22]. **frameworks** [WP20]. **Free** [BBC20, CLS⁺20, FMFG20, GBM20, JGM21, KK23, MXM20, Min20, NNT⁺20, SZLD20, ZK21, AQMM⁺23, BF22, BCN22, CSP20, GVJ⁺22, GH22b, GH23, HB21, HBM⁺20, LPF⁺23, MPP23, MN20, MB21, NML21, ÖLP⁺20, PPV⁺21, PDC23, SY21, SCCZ21, SHH⁺23b, SHH⁺23a, TM20, TTK23, TYZ20, WFBB22, WdGG24, YBS⁺20, YIO20, ZQ24]. **Free-energy** [GBM20, KK23, SY21]. **frequencies** [OM23]. **frequency** [IN23a, SZL23]. **frequency-dependent** [IN23a, SZL23]. **friendly** [SKS21, ZK23]. **fromage** [RDS⁺20]. **Front** [AFR⁺24b, CGSP24b, HAC⁺23a, KWMPR24a, SNK24a, WTST24b, WLSC23b]. **frustrated** [FP22, MC24, ZS22]. **FSATOOL** [SWLC22, WLSC23a, ZGZC20]. **Fukui** [GFRNC21, GUCCR20]. **full** [RMJ21, YLZ⁺22]. **fullerene** [AK20, YLZ⁺22]. **fullerenes** [SSSA23, WKCP21]. **Fulleride** [AS23]. **Fulleride-metal** [AS23]. **fully** [LEP⁺21]. **fumarate** [CFOMCB⁺22]. **function** [AV20, BPL⁺22, ĆPP⁺22, IN23b, KFTB20b, KPR23, KDP⁺22, SWF⁺20, Tou21, WMZJ20, YFH⁺21]. **function-based** [AV20]. **function-related** [BPL⁺22]. **Functional** [BBK20, CWZD20, SK20, YXGZ20, APS20, AS21, ABAQ⁺23, BWS20, BA22, Ben22, CFOMCB⁺22, CHVF21, CPG21, Cer22, CMD⁺22, CTBB20,

DRBT24, DZL⁺²⁰, DOT22, FB20, GH22a, GD23, HM21, HCS⁺²⁰, HLV⁺²⁴, IYI⁺²⁰, IW24, KS21, KdILC22, LRF⁺²¹, LSC24, MWK⁺²⁰, MNH21, MLB⁺²³, MFS22, MKB⁺²¹, MGCM21, MH20, MSE⁺²¹, MSS20, NEG⁺²⁰, NN20, OTZW24, OE20, OMC⁺²⁰, OAN⁺²³, PCB⁺²⁴, RC22, RMBSPJSG24, SDK20, dASRHB21, SC22, SSYB⁺²⁰, SZP⁺²⁰, TANC23, TLS23, WKCP21, ZHHS21, ZHG⁺²⁴, ZGZ⁺²⁰]. **functionalization** [SBFSJMLU23].

Functionalized [LR20, FP23, HCY⁺²², KGS⁺²¹, KJV23, dCB23, YYZ⁺²¹]. **functionals** [BOPJ^{+21a}, DK23, GAP21, HMK23, HM21, HCS⁺²⁰, MH22, MN20, MKK⁺²², NG20, RMJ21, TV22, WS21]. **Functions** [GJMPB⁺²⁰, CC22, CKH23, CV22, GUCCR20, IN23b, Kop22b, MAM⁺²³, MEKH22, MFS22, MCP23, SM20, SCZ⁺²¹, TAC⁺²³]. **further** [BXY⁺²⁴]. **fused** [BMA⁺²⁴]. **fusion** [CGSP24a, EIT⁺²¹]. **future** [IRB⁺²³]. **Fuzzy** [GJMPB⁺²⁰, GJMPVR⁺²⁰].

G [BWM20, CDCT21, CD20, WGKG20]. **G-protein** [WGKG20]. **G-Protein-Coupled** [BWM20]. **G3B3** [SW21]. **G4** [SW21]. **Ga** [AS20]. **GalaxyDock2** [LYKS23]. **GalaxyDock2-HEME** [LYKS23]. **gallic** [KK22a]. **GAMaterial** [LHH⁺²³]. **gamble** [GNL⁺²²]. **gap** [PGDD24]. **Gas** [OM23, AZKM22, APR21, DC22b, IMT⁺²¹, KGS⁺²², MSYS23, Mon24, MK22b, SW21, WG20, YSMS24]. **Gas-phase** [OM23, AZKM22, DC22b, IMT⁺²¹, SW21]. **gases** [YMSS23]. **Gaussian** [AAL21, BP22, GRN20, GH22b, GH23, IN23b, LB21, LB22, MP24, SS23, SLB23]. **Gaussians** [ALA20]. **GDIS** [VWFR21]. **Ge** [LXP⁺²², WMJ⁺²², Wan23, ZWL^{+24a}, GPM21b, SGT⁺²⁰, WTST24a]. **General** [Gao20, BA24, RMJ21, UKBD23, VCL20]. **general-purpose** [BA24]. **Generalized** [GCL⁺²⁰, HTFY21, IWN24, SH23, VV20b, BMT⁺²¹, JKS23, LWF⁺²², NG20, XCJ20]. **Generalized-ensemble** [HTFY21]. **generate** [AG21]. **generated** [WKG⁺²³]. **Generating** [SHM⁺²⁰, VAP⁺²¹]. **Generation** [MC24, AMF⁺²⁰, Che23, DYGM21, EVKL21, Gao20, GSD⁺²², JGK⁺²², LYX⁺²², Nee23, PRIP24, RB22, SM22a, dSSCC24, TIK21]. **generative** [PMT⁺²²]. **generic** [WFBB22]. **genetic** [LHH⁺²³, RDB23, SS20]. **genetic-algorithm** [LHH⁺²³]. **Geometric** [ETT21b, OAC23, DHD21]. **Geometrical** [RLHG⁺²³, GJMPVR⁺²⁰, KTM⁺²³, LWC⁺²⁴]. **geometrically** [PFP⁺²¹]. **Geometries** [LXP⁺²², NG20, WD20]. **Geometry** [LPP20, SBD⁺²¹, AZKM22, CMD⁺²², LLS22a, LL21b, MMK⁺²⁰, OC23]. **germa** [KDMM24]. **germaboryne** [DDSM23]. **Ge** \equiv [DDSM23]. **GFN** [MKB⁺²¹, OM22]. **GFN-xTB** [MKB⁺²¹]. **GFP** [RPD^{+20a}]. **giant** [WKCP21]. **GIAO** [MPOC21]. **GIAO-NMR** [MPOC21]. **glassy** [Tou21]. **Glioblastoma** [CM20b]. **Global** [CPG21, AZKM22, DC22a, MZ21, NAAP21, OC23, OKI⁺²¹, RTB23, TTH^{+21a}]. **Glucopyranose** [Mon24]. **glucose** [DOT22]. **Glycans** [KUNT20]. **glycine** [HB21, ONC20]. **glycoprotein** [ONA⁺²⁰]. **glycoprotein-enhanced** [ONA⁺²⁰]. **glycosaminoglycan** [MGB⁺²²]. **glycosaminoglycans** [MZMK⁺²¹]. **goal**

[NSRK21]. **goal-oriented** [NSRK21]. **GoGreenGo** [PKT21]. **gold** [LL21a, NST⁺20, NSKN21, POPGS22]. **GPRI** [BA24]. **GPU** [ZKJ⁺23]. **GPU-specific** [ZKJ⁺23]. **gradient** [BMT⁺21, LC22, NG20, VV20b]. **gradients** [BSF20, VCL20]. **grafted** [Che23, GBM20]. **Grained** [MT20a, WSL⁺20, WZZ⁺20, BS23, CST23, GWN21, IL24, KGTL21, LL21b, LL22, MT19, SSDL⁺23]. **grand** [GGK20, ZKJ⁺23]. **grand-canonical** [GGK20]. **Graph** [CR24, BCN22, CdSB⁺21, NGD22, RSHG23, SKY24, WCY⁺24]. **Graph-based** [CR24, RSHG23]. **Graphene** [KK22c, BWS20, DZL⁺20, DOT22, RC22, SS23, SPT21, dSSCC24, YC20, dCRM21]. **Graphene-induced** [KK22c]. **graphene-supported** [BWS20, DZL⁺20]. **Graphical** [SBG20, MLG⁺21b]. **Graphics** [GCL⁺20, DWZ22]. **Graphs** [SBG20, DHD21, YGG⁺23]. **grasp** [BPDG21]. **greater** [LML⁺23]. **green** [AQIS⁺24]. **Gremlin** [CM20b]. **Gremlin-1** [CM20b]. **Grid** [Min20, CP23, RB24]. **grid-based** [CP23]. **GROMACS** [LKM20, MPP23]. **Ground** [Ari24, KWB24, Kop22b, BGPR24, HPM⁺21, KBHG23, WD20]. **Ground-state** [Kop22b, KBHG23, WD20]. **Group** [LXP⁺22, SBG20, BPL⁺22, BD22, BBK⁺21, Brz22, DPSG20, GPM21b, KW22, Klo22, KBHG23, LGM22, NUK21, PB20, PT21, PLZT23, PP23, RMJ21, THH⁺24, TANC23, TT20, WCD⁺23, XSP⁺23, ZS22, ZHG⁺24, SMH21]. **Group-14** [LXP⁺22]. **group-CASPT2** [TT20]. **group-modified** [ZHG⁺24]. **groups** [CCZ23, HPG20]. **Growth** [XDZ23, BHR⁺21]. **GRP1** [PT20]. **guanidine** [RLHG⁺23]. **guanidine-quinoline** [RLHG⁺23]. **guanine** [XZX⁺22, BVGB23]. **guanosine** [XZX⁺22]. **guest** [BRNB21, GBM20, MJS⁺23, YLZ⁺22]. **guest-guest** [MJS⁺23]. **guests** [KPKS23]. **GUI** [KLP⁺22, QLC⁺20, SSMP23]. **Guide** [ARR22a, SSMP23]. **Guided** [CLS⁺20, CGSP24a, CBK⁺24]. **Gulari** [VFCG20].

H [KPTT21, LR20, PGP⁺23, TTK23, WSV20, AKGD24, AWK⁺23, GAP21, GJL21, KPTT21, KM24, LML⁺23, LL21b, MCP23, MBBU23, OKI⁺21, THH⁺24, YYS20, ZHHS21, dCVARN20]. **H-BEE** [AKGD24]. **H-bonded** [LML⁺23]. **H/D** [dCVARN20]. **H10N7** [SSPK24]. **hairpin** [YFH⁺21, ZZ23b]. **half** [SS24]. **halide** [APR21, dARW⁺23]. **halides** [AQMM⁺23]. **haloacetates** [CNF23]. **halogen** [CB20, JGGPN21, SJZ⁺21, ZBH⁺23]. **halogenated** [LK22]. **Hamiltonian** [IK21]. **Hamiltonians** [IWN24, KKAK23]. **Hammett** [dCB23]. **handling** [WHJM23]. **hardness** [GFRNC21]. **harmonic** [CS23, Cer22, EVKL21]. **Hartree** [BTSB22, BBK20, NSH23, NI22]. **harvesting** [AQRA⁺23]. **having** [DC22a]. **HC** [BdLC21]. **HCFC** [dSSRVdM24]. **HCFC-31** [dSSRVdM24]. **HCl** [AWK⁺23]. **HCVpred** [MPuS⁺20]. **HD** [BBY⁺21]. **HDAC** [MIK⁺23]. **HDAC2** [MIK⁺23]. **HDAC2-selectivity** [MIK⁺23]. **H...** [ARR22b]. **heat** [BAO⁺20, SSYB⁺20]. **heat-shock** [BAO⁺20]. **heatbath** [UR23]. **heatbath-CI** [UR23]. **heavy** [DART21, Klo22, ZWL⁺24a]. **Hedgehog** [Ban20]. **Heisenberg** [KKAK23]. **helical** [MVV22, SSS⁺20b]. **helicenes**

[LLJ⁺24]. **helices** [VCL20]. **helium** [BGS⁺20]. **Helix** [MKSS20, HTFY21, NYM22]. **helix-mimetic** [HTFY21]. **heme** [LYKS23, SWF⁺20, SWM⁺20b, LYKS23]. **hemodialysis** [MSA22a]. **hemoproteins** [FAK24]. **hepatitis** [MPuS⁺20]. **heptagons** [IW23]. **Herzberg** [Tou21]. **hetero** [GPM21b]. **hetero-bileptic** [GPM21b]. **heterobimetallic** [ZMH⁺21]. **heterocycle** [LLJ⁺24]. **heterocycles** [BSS⁺22]. **heterocyclic** [FP22, JGSA22]. **heterointerface** [SZP⁺20]. **heterojunction** [TANC23]. **Heterolytic** [LR20]. **heteronuclear** [KW22, SJZ⁺21]. **heteroporphyrins** [SaATR24]. **heterostructures** [PSM⁺20]. **Heusler** [SS24]. **hexa** [FDK22]. **hexa-** [FDK22]. **hexagonal** [NDK24]. **hexane** [NS22]. **Hf** [DBE20, AWK⁺23]. **Hg** [SSS⁺20a]. **hidden** [GM22, SSP23]. **Hierarchical** [NN20, dASRHB21, AÄFJ21, BTC24, LMPT21]. **High** [BLB20, EVKL21, KUNT20, LCP24, NBE⁺23, OKI⁺21, BSF20, DK23, GWN21, GVJ⁺22, IAF⁺24, KE23b, KWX23, KGG21, KDP⁺22, LHC⁺21, MZ21, PPV⁺21, RD23, XLW⁺22, ZWL24b]. **high-level** [BSF20]. **High-order** [EVKL21]. **High-performance** [BLB20]. **high-polarity** [DK23]. **high-resolution** [IAF⁺24]. **high-speed** [GWN21]. **High-throughput** [NBE⁺23]. **Higher** [HFPS20]. **highest** [KPHV23, LJW⁺23]. **highlight** [SNK24b]. **Highly** [JFZ⁺20, SHH⁺23b, SHH⁺23a]. **Hirshfeld** [LC22, MSE⁺21]. **histidine** [FAK24]. **histogram** [MT20b]. **HIV** [CBK⁺24, GG22, NPGP23, PWX⁺20, WCT⁺23]. **HIV-1** [CBK⁺24, PWX⁺20, WCT⁺23]. **HMX** [ZG21]. **Hoff** [ZXD20b, ZXD20a]. **Hoff/Le** [ZXD20b, ZXD20a]. **Hole** [RZS⁺23, JGGPN21, LK22, Sch22a, SJZ⁺21]. **HOMO** [CMD⁺22]. **HOMO-LUMO** [CMD⁺22]. **homodimeric** [DPSG20]. **homology** [CFOMCB⁺22]. **Homolytic** [LR20]. **hoops** [FDD⁺23]. **HOPO** [SDK20]. **Hopping** [YXGZ20, FCPG20]. **host** [BRNB21, GBM20, MJS⁺23, PPRS22, YLZ⁺22]. **host-guest** [BRNB21, GBM20, MJS⁺23, YLZ⁺22]. **hosts** [KPKS23]. **hot** [KSS21b, KSRB⁺21]. **HRas** [XZX⁺22]. **Hubbard** [POPGS22, TLD⁺22]. **huge** [JKK⁺21]. **Human** [KUNT20, KLZ⁺23, LSC⁺23, SCCZ21]. **human-norovirus** [LSC⁺23]. **Hybrid** [CdSB⁺21, ZK21, AR20, BOPJ⁺21a, Che23, FV20, HMK23, HUO23, KGS⁺21, MN20, MKK⁺22, NG20, RPD⁺20a, RMBSPJSG24, SS20, SZP⁺20, WKD⁺21, XZW⁺21, YW20]. **hybrids** [CPG21, HSG21, OMC⁺20]. **hydrate** [MJS⁺23]. **hydrated** [YC20]. **hydrates** [VCRP23]. **Hydration** [ALA⁺22, HS22, KPTT21, PCI23, KK23, TTK23, YIO20]. **hydrazine** [PFP⁺21]. **hydride** [GSSG24, MC24]. **Hydrides** [PWW20]. **Hydrido** [SLML24]. **hydroalkylation** [BXY⁺24]. **hydrocarbon** [NS22]. **hydrocarbons** [GAP21]. **Hydrocyanation** [JFZ⁺20]. **Hydrogen** [AKGD24, HS23, SKKG22, AV20, ARR22b, AD23, BCN22, CVGVN⁺20, ČNF23, CL23, CB20, DHN⁺21, DLH⁺23, GJL21, GH22b, KPTT21, KZ24,

LKT21, NTK21, SGGG22, SS23, SJZ⁺21, SD21, TTT⁺21, ZFRM20].
hydrogen/halogen [SJZ⁺21]. **hydrogenation** [ZZG⁺21]. **Hydrolysis**
 [JWS⁺24, PDP⁺24, ZLLL22]. **hydrophilicity** [MSA22a]. **hydrophobic**
 [KPKS23]. **Hydrostatic** [SL20]. **hydroxychromones** [AIV20].
hydroxylation [HYA⁺20, MNH21]. **hydroxymethyl** [MSA22a].
hydroxyquinolinato [AS20]. **hydroxyquinolinone** [SEBE21]. **hyper**
 [MAI22]. **hyper-softness** [MAI22]. **hypercoordinate** [YrYqLhC23].
Hypercube [Bal20a]. **hypericin** [DMTR22]. **Hyperplanes** [Bal20a].
hypervalent [SCZ⁺21].

I/II [RLHG⁺23]. **ICI** [PLT24]. **icosahedral** [PGP⁺23]. **idea** [BBB⁺23].
Identification [PPP21, RDK⁺22, LCP21, MSE⁺21]. **identified** [SSYB⁺20].
identify [KDP⁺22, LKK⁺23, Sch22b, SYS⁺21, WRVP22]. **Identifying**
 [PAS⁺20]. **if** [RD24]. **IGMP** [LKK⁺23]. **II** [ABZ20b, AD20, GP21,
 SVDS21, SSS⁺20a, WYC⁺24, YYS20, GH22a, KLC⁺24, KI24, RLHG⁺23].
II-Importance [KLC⁺24]. **III** [AS20, HRTSS⁺20, KKAK23, RLHG⁺23].
ILE [MPOC21]. **illustrated** [BCN22]. **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, BUNO22a, BBC⁺21b, BOPJ⁺21b, CX21a, ETT21a, GPM21a,
 GKA⁺23a, KFTB20a, KSS21a, KK22b, MLG⁺21a, QLW⁺22a, RPD⁺20b,
 SWM⁺20a, dRHB21, SSFS22a, TTH⁺21b, TCS⁺21b, VV20a]. **images**
 [QLW⁺22b]. **imaging** [Yos24]. **Imidazole** [CFOMCB⁺22, SKT24].
imidazopyridine [ZOD⁺22]. **imino** [YFS20]. **immersive** [MSL⁺20].
Immunodeficiency [KUNT20]. **Impact**
 [MLM⁺24, KDKS21, OTZW24, OM23, SPSH20, VCRP23]. **impacts**
 [MVV22]. **impedance** [KF24]. **Implementation**
 [HAC⁺23b, NP23, PDP⁺24, YLZ⁺20, BPT⁺23, CSGVF⁺20, CPG21, FR21,
 HGR⁺24, OMC⁺20, SSDL⁺23]. **implementations** [CHVF21]. **implications**
 [KSP21]. **Implicit** [GRBN21, GCL⁺20, CCHS23, RPD⁺20a]. **Importance**
 [HKS20, DSB23, KLC⁺24]. **important** [SGGG22]. **improbability**
 [RLR⁺20]. **Improved** [BBK20, LJ20, CX21b, DKB23, RTB⁺22, ZKJ⁺23].
Improving [FB20, MKK⁺22, PNT⁺22, SZP⁺20, YFH⁺21, FYIO23].
in-silico [dMBdAVdS24]. **in-situ** [MC24, WKG⁺23]. **inactivation**
 [RPA⁺24]. **includes** [VWJ23]. **including** [FBP⁺22]. **inclusion** [YLZ⁺22].
Incorporating [BTC24, Gie21]. **incorrectly** [GAP21]. **increase** [LKM20].
increases [HREvdK⁺20]. **indenotetracene** [CCPR24]. **Independent**
 [LC22, CSG⁺21, LGC21, WFBB22]. **index** [PC23, Sch22b]. **Indexes**
 [WZZ⁺20, KdLLC22]. **indicator** [BA24]. **individual** [AD23, BRNB21].
INDO [Gie21]. **INDO/S** [Gie21]. **Induced**
 [QB20, CCPR24, EK20b, EK20c, FVSS20, KK22c, SCC⁺22, TTH⁺21a].
inexpensive [Ben22]. **Influence**
 [GAG20, MCP23, PT21, SGGG22, Brz22, CCHS23, SVDS21, SKT24].

influenza [SSPK24, SSS+20b]. **Information**

[Ano20-29, Ano20-30, Ano20-55, Ano20-56, Ano20-57, Ano20-58, Ano20-59, Ano20-60, Ano20-31, Ano20-32, Ano20-33, Ano20-34, Ano20-35, Ano20-36, Ano20-37, Ano20-38, Ano20-39, Ano20-40, Ano20-41, Ano20-42, Ano20-43, Ano20-44, Ano20-45, Ano20-46, Ano20-47, Ano20-48, Ano20-49, Ano20-50, Ano20-51, Ano20-52, Ano20-53, Ano20-54, Ano21a, Ano21b, Ano21z, Ano21-27, Ano21-28, Ano21-29, Ano21-30, Ano21-31, Ano21-32, Ano21c, Ano21d, Ano21e, Ano21f, Ano21g, Ano21h, Ano21i, Ano21j, Ano21k, Ano21l, Ano21m, Ano21n, Ano21o, Ano21p, Ano21q, Ano21r, Ano21s, Ano21t, Ano21u, Ano21v, Ano21w, Ano21x, Ano21y, Ano22a, Ano22b, Ano22-27, Ano22-28, Ano22-29, Ano22-30, Ano22-31, Ano22-32, Ano22c, Ano22d, Ano22e, Ano22f, Ano22g, Ano22h, Ano22i, Ano22j, Ano22k, Ano22l, Ano22m, Ano22n, Ano22o, Ano22p, Ano22q].

Information

[Ano22r, Ano22s, Ano22t, Ano22u, Ano22v, Ano22w, Ano22x, Ano22y, Ano22z, Ano23a, Ano23b, Ano23-27, Ano23-28, Ano23-29, Ano23-30, Ano23-31, Ano23-32, Ano23c, Ano23d, Ano23e, Ano23f, Ano23g, Ano23h, Ano23i, Ano23j, Ano23k, Ano23l, Ano23m, Ano23n, Ano23o, Ano23p, Ano23q, Ano23r, Ano23s, Ano23t, Ano23u, Ano23v, Ano23w, Ano23x, Ano23y, Ano23z, Ano24b, Ano24c, Ano24d, Ano24e, Ano24f, Ano24g, Ano24h, Ano24i, Ano24j, Ano24k, Ano24l, Ano24m, Ano24n, Ano24o, Ano24p, Ano24q, Ano24r, Ano24s, TAC+23].

information-theoretic [TAC+23]. **infrared**

[GPEK+20, KGS+22, LZW+23, PGP+21]. **Ingenuity** [FYIO23].

ingredients [MBBU23]. **inhibition** [dSCCN21, YC23]. **inhibitor**

[BAO+20, BVC+23, EIT+21, GG22, MIK+23]. **inhibitors**

[CFOMCB+22, CGSP24a, KI24, KGD+21, MPuS+20, PWX+20, PPP21, PPRS22, RKC21, RDK+22, SKL23, TWT+22, ZOD+22]. **inhibitory**

[BHR+21]. **inhibits** [HTFY21]. **inhomogeneous** [RB24]. **initial** [AAID22].

Initio [GK24, SK20, VAL20, AST24, BSS+22, BBC+21a, BBBP+23, DC22b, ERVN24, FCB23, GP21, KPTT21, Kop22a, KGD+21, MAM+23, MN20, PCB+24, PGP+23, PLT24, RZS+23, RPD+20a, dASRHB21, SPSH20, SNN+21, WTST24a, XSP+23, KRSD+23, LCLB24]. **inner** [Sán20].

inner-shell [Sán20]. **inorganic** [Brz22, KGS+21, KS21, SZP+20]. **input**

[GSD+22, VAP+21]. **inputs** [HREvdK+20]. **inserted** [LZW+23]. **Insight**

[JFZ+20, KPHV23, MK22b, DGM22, HRTSS+20, YJZ+22]. **Insights**

[ASL+20, BRNB21, BAM+24, DSS+24, FLT23, GOY20, KS24, MNH21, OTZW24, SAZ+23, SZP+20, CP23, KFLP21, MML+23, PPRS22, TAB+24, VT24]. **inspired** [MSA22a]. **Instanton** [SRB21]. **insulator** [EK20b].

insulator-to-metal [EK20b]. **integral** [Gao20, Nee23, SCvW22, Shi22].

integrals [DWZ22, IN23a, IN23b]. **Integrated**

[BBB+23, VDK+20, MLG+21b, SWLC22]. **Integration**

[VWFR21, KCGK20]. **intelligence** [DPY+22, KI24]. **intensities** [TTT+21].

intensity [GAP21]. **inter** [BOPJ+21a]. **inter-molecular** [BOPJ+21a].

interacting [CSGVF+20, JCMHT22, JGGPN21, OE20, TPZ+20].

Interaction

[KUNT20, MBBU23, PT20, dCRM21, AR24, AA20, ASW20, BdLC21, CV22, CSWW20, COK22, GKO⁺²², HTTT23, HTFY21, IN23a, Jab22b, KWYN23, KLZ⁺²³, MAM⁺²³, MR21, MPR22, MEKH22, NI22, PHS⁺²⁰, QLW^{+22b}, SM23, TWT⁺²², TTK23, VCRP23, WMZJ20, WKL22, YOCMA23, YLZ⁺²²]. **interaction-site** [KWYN23]. **Interactions** [BWM20, LJ20, WP20, BW22a, BS23, BRNB21, BPDG21, CM20b, CTBB20, ERVN24, EPT21, FDD⁺²³, FM21, HPG20, HTFY21, IL24, Klo22, KZ24, KKAK23, KGD⁺²¹, LKK⁺²³, LEP⁺²¹, LC22, MJS⁺²³, ODL20, OE20, PDC23, RZS⁺²³, RMJ21, SAZ⁺²³, SI22, SKT24, dSSCC24, YW20]. **Interatomic** [AA20, ZFRM20]. **intercalation** [HKS20, SGG22]. **interest** [MLGY24]. **interesting** [HPG20]. **interface** [ABNG22, CCZ23, DMD⁺²¹, SNN⁺²¹]. **interfacial** [CM20a]. **intermediate** [MMK⁺²⁰]. **Intermediates** [SK20, DSB23, LHG⁺²³]. **Intermolecular** [KGD⁺²¹, OOO20, BSS⁺²², HTFY21, LLZ⁺²³, MGCM21, RZS⁺²³, SI22]. **Internal** [WZZ⁺²⁰, ABTM22, BLB20, KZJ22]. **interoperable** [BPT⁺²³]. **Interplay** [HYA⁺²⁰, ZRS20]. **Interpolation** [WSL⁺²⁰, GWN21]. **interpretable** [BK22]. **Interpretation** [LCC⁺²¹]. **interpreter** [PSGL21]. **intersection** [AIV20]. **Interstitial** [PGP⁺²¹]. **intersystem** [SaATR24, WTST24a]. **intra** [BOPJ^{+21a}]. **intra-** [BOPJ^{+21a}]. **Intramolecular** [FM21, ARR22b, AIV20, CRT⁺²¹, FP22, KSP21, dCB23, RA20]. **intricacies** [JWS⁺²⁴]. **Intrinsic** [AD20, MLGY24]. **intrinsically** [SY21]. **Introducing** [SKS21]. **invariant** [KSRB⁺²¹, OKK22]. **inverse** [LBH⁺²²]. **inversion** [SWF⁺²⁰, SWM^{+20b}]. **Investigating** [BSL20, Nan24]. **Investigation** [CSP20, ĆPP⁺²², DOT22, HL20, AQMM⁺²³, AST24, BBBP⁺²³, DHN⁺²¹, FBM⁺²³, KPTT21, KMR⁺²⁴, KDKS21, KJV23, KK22a, MKB⁺²¹, NMCM21, RPA⁺²⁴, SS20, SS24, SKGG23, SLML24, ZS22, ZWL24b]. **investigations** [AKGD24, BMA⁺²⁴, RZS⁺²³]. **involved** [CRT⁺²¹]. **Involving** [SK20, KZJ22, SJZ⁺²¹, SBB⁺²², ZBH⁺²³]. **IOData** [VAP⁺²¹]. **Iodido** [SVDS21]. **Iodine** [ASL⁺²⁰, DMTR22, SCZ⁺²¹]. **iodine-containing** [DMTR22]. **Iogansen** [TTT⁺²¹]. **Ion** [SLR⁺²⁰, CX21b, FVSS20, HPG20, JRS20, LA20, OM23, dSSCC24, dSSRVdM24, XAD20, YJZ⁺²²]. **ion-induced** [FVSS20]. **Ion-Pair** [SLR⁺²⁰, dSSRVdM24]. **Ionic** [VAL20, AÅFJ21, Cer22, IAS⁺²⁴, LWF⁺²², LEP⁺²¹, SI22, XAD20]. **Ionization** [MLGY24, ALA20, HNCL24, MLB⁺²³]. **ionizations** [KM24]. **ions** [KEK23, ODL20, SDK20, YC20]. **IR** [TTT⁺²¹, DZL⁺²⁰]. **Iron** [FAK24, CL23, GKA^{+23b}, Jab22b, KKAK23, SHP⁺²³]. **Iron-histidine** [FAK24]. **irradiation** [LYX⁺²²]. **Irreducible** [Bal20a]. **isodesmic** [WKCP21]. **isodesmic-type** [WKCP21]. **Isoelectronic** [ZXD20a, Ano24a, SVTK⁺²², SK23, ZXD20b]. **isolable** [FNPD22]. **isolated** [CA22, IW23, JS21, LML⁺²³]. **Isolation** [BLP20, LRKD23]. **isoleucine** [MPOC21]. **isomerase** [DPSG20]. **Isomerism** [PYA24]. **isomerization** [GK24, OKI⁺²¹]. **isomers** [OKI⁺²¹, ONC20]. **isothermal** [LL21a]. **isotope** [JMK⁺²⁰, dCVARN20]. **isotopologues** [SR23]. **iSPECTRON** [SNN⁺²¹].

Issue [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, Ano20-29, Ano20-30, Ano20-55, Ano20-56, Ano20-57, Ano20-58, Ano20-59, Ano20-60, Ano20-31, Ano20-32, Ano20-33, Ano20-34, Ano20-35, Ano20-36, Ano20-37, Ano20-38, Ano20-39, Ano20-40, Ano20-41, Ano20-42, Ano20-43, Ano20-44, Ano20-45, Ano20-46, Ano20-47, Ano20-48, Ano20-49, Ano20-50, Ano20-51, Ano20-52, Ano20-53, Ano20-54, Ano21a, Ano21b, Ano21z, Ano21-27, Ano21-28, Ano21-29, Ano21-30, Ano21-31, Ano21-32, Ano21c, Ano21d, Ano21e, Ano21f, Ano21g, Ano21h, Ano21i, Ano21j, Ano21k, Ano21l, Ano21m, Ano21n, Ano21o, Ano21p, Ano21q, Ano21r, Ano21s, Ano21t]. **Issue** [Ano21u, Ano21v, Ano21w, Ano21x, Ano21y, Ano22a, Ano22b, Ano22-27, Ano22-28, Ano22-29, Ano22-30, Ano22-31, Ano22-32, Ano22c, Ano22d, Ano22e, Ano22f, Ano22g, Ano22h, Ano22i, Ano22j, Ano22k, Ano22l, Ano22m, Ano22n, Ano22o, Ano22p, Ano22q, Ano22r, Ano22s, Ano22t, Ano22u, Ano22v, Ano22w, Ano22x, Ano22y, Ano22z, Ano23a, Ano23b, Ano23-27, Ano23-28, Ano23-29, Ano23-30, Ano23-31, Ano23-32, Ano23c, Ano23d, Ano23e, Ano23f, Ano23g, Ano23h, Ano23i, Ano23j, Ano23k, Ano23l, Ano23m, Ano23n, Ano23o, Ano23p, Ano23q, Ano23r, Ano23s, Ano23t, Ano23u, Ano23v, Ano23w, Ano23x, Ano23y, Ano23z, Ano24b, Ano24c, Ano24d, Ano24e, Ano24f, Ano24g, Ano24h, Ano24i, Ano24j, Ano24k, Ano24l, Ano24m, Ano24n, Ano24o, Ano24p, Ano24q, Ano24r, Ano24s]. **Issue** [RPD⁺20b]. **iterative** [VV21]. **IV** [CMD⁺22, PPSP20, SVDS21].

J [MT20a, WG21]. **Jahn** [PGDD24, PDL24]. **JAK2** [SKL23]. **jcc.25747** [MT20a]. **Jones** [SG20]. **Judicious** [YYZ⁺21]. **JunChS** [DKB23]. **JunChS-F12** [DKB23].

kernel [CdSB⁺21]. **kesterites** [MZ21]. **ketenylidene** [LZW⁺23]. **Keto** [LKAT22]. **Keto-enol** [LKAT22]. **keV** [KM24]. **Key** [VV20b, FM21, PPRS22, TANC23]. **kinase** [SNW22, TWT⁺22]. **kinase-2** [TWT⁺22]. **kinematic** [HC21]. **kinetic** [EG20, JMK⁺20, MIK⁺23, SaATR24, VHS⁺24, WKG⁺23, dCVARN20]. **Kinetics** [SK20, CGMRVBAl22, CD20, DWSX20, RMJ21, SNW22, ZLLL22]. **kinks** [MA23b]. **Kohn** [BTSB22, EK20a, HCS⁺20, MB21]. **Koopmans** [GX20]. **KScF** [PDL24]. **Kunitz** [BVC⁺23]. **Kunitz-type** [BVC⁺23]. **Kylin** [XSP⁺23].

L [CK22, OSM20, ZWY⁺22]. **L-lactide** [OSM20]. **L-OPLS** [ZWY⁺22]. **L-W1X** [CK22]. **L2MC** [NML21]. **L536S** [CSP20]. **lab** [SC23]. **labels** [FYIO23]. **lactamase** [KGD⁺21]. **lactide** [OSM20]. **LaFeO** [TAB⁺24]. **Lagrangian** [UYJ⁺24]. **lambda** [ZQ24]. **landscape** [BBC20, SY21, YYS20]. **landscapes** [GVJ⁺22, PPV⁺21]. **Langevin** [SH23]. **language**

[DGS24, WCY⁺24]. **Lantern** [LLKS23]. **Lantern-type** [LLKS23]. **lanthanides** [ALA⁺22, SLB23]. **Laplacian** [TTDT20]. **Large** [MFC20, NS22, UAC⁺23, AD23, AKGD24, BTC24, CJHW21, JKS23, KS21, KWX23, RBM⁺23, SSDL⁺23, UR23]. **large-scale** [BTC24, CJHW21]. **Large-Sized** [MFC20]. **laser** [LYX⁺22, LAM⁺23, MLX⁺24, SCC⁺22]. **laser-induced** [SCC⁺22]. **Late** [PWW20]. **LaTiO** [PGDD24]. **lattice** [NMF121]. **layer** [YrYqLhC23]. **layered** [EK20c]. **layers** [LMPT21]. **lead** [AQMM⁺23, dMBdAVdS24]. **lead-free** [AQMM⁺23]. **Leading** [AD20, NG20]. **leapfrog** [MIP⁺21]. **learned** [OTZW24]. **Learning** [LPP20, SKY24, BP22, CdSB⁺21, CBK⁺24, COK22, DGS24, HBT⁺20, HLV⁺24, JGK⁺22, KM22, KF24, KB22, KDP⁺22, LHB⁺24, MLC⁺23, MYYS24, NGD22, PSW⁺24, PDP⁺24, RDB23, RD24, SKL23, TXJT23, TCS⁺21a, VT24, WRBT21, WYC⁺24, WLSC23a, XZC⁺24, YFS20, Yos24]. **learning-assisted** [RD24, WRBT21]. **learning-guided** [CBK⁺24]. **length** [FR21, MVP⁺20]. **Lennard** [SG20]. **Lennard-Jones** [SG20]. **less** [CSWW20]. **leucine** [CGMRVBAI22]. **leucoindigo** [PPFL23]. **level** [ABNG22, BSF20, JK21, PHS⁺20]. **levels** [ERVN24, Kop22b]. **Lewis** [Brz23, FP22, HLV⁺24, MC24, NMCM21, OE20, PT21, PLZT23, ZS22]. **Li** [JX24, LEP⁺21, Ore24]. **Li-molecule** [Ore24]. **Libkrylov** [RBM⁺23]. **library** [JGK⁺22, KRSD⁺23, RBM⁺23, RDS⁺20, VAP⁺21, WHJM23]. **Lif** [VDK⁺20]. **lifetime** [FCB23]. **Ligand** [Ban20, JFZ⁺20, KW22, MXM20, NNT⁺20, AAe20, BTC24, BKM21, HGF20, IK21, KDLP21, KK23, KDP⁺22, LYKS23, MAKZ23, Ngo21, ÖLP⁺20, OM23, PMT⁺22, PNT⁺22, PSB⁺22, SNW22, TWT⁺22, TTK23, VWP⁺22, WCD⁺23, YIO20, ZOD⁺22]. **ligand-alkali** [OM23]. **ligand-based** [PMT⁺22]. **Ligand-Binding** [NNT⁺20, HGF20, Ngo21]. **ligand-free** [YIO20]. **ligand-ranking** [PNT⁺22]. **Ligand-stabilized** [KW22]. **Ligands** [Min20, SZLD20, DDSM23, GPM21b, LLKS23, RvWH23, SVDS21, TLS23]. **lignin** [BW22a]. **like** [DYG21, LSC⁺23, SAZ⁺23, YMSS23]. **limit** [CVGVN⁺20, SCKH21]. **limitations** [TZS⁺22]. **Limiting** [Cha24]. **limits** [WFBB22]. **LIMONADA** [CBB⁺21]. **linear** [OKK22, Sch22a, SNN⁺21, Tou21]. **linearized** [NSRK21]. **linearly** [BMA⁺24]. **link** [GH22a, KGTL21]. **linker** [GJL21]. **Links** [GFRNC21]. **LIO** [SDK20]. **Lipase** [VDK⁺20]. **lipid** [KFTB20b, WRBT21]. **lipids** [IL24, KCF⁺20]. **lipophilicity** [HS22]. **liquid** [CCZ23, IAS⁺24, KGS⁺22, LEP⁺21, MMF⁺24, SPSH20, ZWY⁺22]. **liquid-IAS⁺24**. **liquid-based** [LEP⁺21]. **Liquids** [VAL20, BUNO22b, Cer22, LWF⁺22, SI22, TPD21]. **lithium** [HM21, KE23b, Kop22b, Mil21, dSSCC24, SGT⁺20]. **lithium-based** [HM21]. **lithium-chloride** [Mil21]. **LLS** [GKO⁺22]. **LLS-SC** [GKO⁺22]. **load** [DLH⁺23]. **LOBSTER** [NEG⁺20]. **Local** [NEG⁺20, PKT21, SPT21, WSV20, BEKM24, DTA21, FB21, FDK22, FAK24, GFRNC21, HMK23, MAI22, PW20, TV22, VV20b]. **localization** [BMT23, LT23, WFLZ23]. **localized** [CdSB⁺21]. **locating**

[SDH23, XZC⁺24]. **logarithm** [SHH⁺23b]. **Lone** [TTDT20]. **Long** [BBK20, LSC⁺23, AS21, CHVF21, GAP21, HTTT23, HTFY21, HCS⁺20]. **Long-range** [BBK20, AS21, CHVF21, GAP21, HTTT23, HTFY21, HCS⁺20]. **Long-time** [LSC⁺23]. **look** [NSKN21]. **lookup** [GWN21]. **loop** [LLS22a, SSPK24]. **loops** [OC23]. **LOV2** [XIV⁺24]. **low** [BBY⁺21, CK22, IK21, KWX23, LWLC21, MdSJ⁺23, OM23, RD24, SM22b]. **low-cost** [CK22]. **low-lying** [IK21, MdSJ⁺23]. **low-symmetry** [SM22b]. **Löwdin** [ASW20]. **lowest** [BGPR24, FCB23]. **lowest-lying** [BGPR24]. **LSL** [FR21]. **LSL-BFGS** [FR21]. **LSLOpt** [FR21]. **Lu** [SLB23]. **LUMO** [CMD⁺22]. **LuMSb** [SS24]. **lutidine** [TYZ20]. **lying** [BGPR24, IK21, MdSJ⁺23].

M [AS20, HSG21, MH20, PPP21, ZMH⁺21, AS20, MH20, PTP23, PP23, SS24, WTST24a, ZMH⁺21]. **Machine** [CBK⁺24, KF24, MLC⁺23, OTZW24, RD24, CdSB⁺21, COK22, DGS24, HBT⁺20, HLV⁺24, KM22, KB22, KDP⁺22, MYYS24, NGD22, PSW⁺24, PDP⁺24, RDB23, SKL23, TCS⁺21a, VT24, WRBT21, WYC⁺24, YFS20]. **Machine-learned** [OTZW24]. **Machine-learning** [MLC⁺23, KDP⁺22]. **Macroscale** [HZG⁺20]. **made** [TPD21]. **magnesium** [ZDBZ20]. **Magnetic** [KKAK23, ABAQ⁺23, LL21b, SBFSJMLU23, TPD21, XDZ23, ZWL⁺24a]. **magnetizabilities** [SZL23]. **magneto** [TAB⁺24]. **magneto-optical** [TAB⁺24]. **maiden** [Jab22b]. **main** [Klo22, PPP21, RMJ21, UAC⁺23, WCD⁺23, YC23]. **main-group** [Klo22, RMJ21, WCD⁺23]. **maleimides** [BAM⁺24]. **manifold** [Yos24]. **Mannose** [KUNT20]. **many** [BMT23, CN21, KSP21, NI22, WFLZ23]. **many-body** [BMT23, KSP21, NI22, WFLZ23]. **many-particle** [CN21]. **Map** [CLS⁺20]. **mapping** [TTDT20]. **maps** [PJJL23]. **Martini** [MT20a, MT21, BAC20, MT19]. **MARVEL** [IAF⁺24]. **Massively** [BBK⁺21, ABTM22, JKS23]. **material** [GGK20, LHH⁺23, MMAZ⁺23, SPT21, SGT⁺20]. **materials** [BEKM24, LRF⁺21, LCP24, LWLC21, PSG21, SAZ⁺23, TV22, ZGZ⁺20]. **Mathematical** [QB20]. **Matrix** [BLP20, BBK⁺21, IW24, RBM⁺23, RA20, TT20, WMZJ20, WHJM23, XSP⁺23]. **matrix-product** [WMZJ20]. **Maximal** [Sch22a]. **maximum** [CTPJH22, TLD⁺22]. **MBAR** [JGM21]. **MBN** [SSFS22b]. **McConst** [SKS21]. **MCML** [BMT⁺21]. **MCO** [GPM21b]. **MD** [CCZ23, FCB23, FBP⁺22, HKFT21, SSS⁺20a, TTK23]. **MDMS** [Zac20]. **Me** [HSG21, SDK20, WLZM20]. **Me-3** [SDK20]. **Mean** [PPV⁺21, VHS⁺24]. **mean-field** [VHS⁺24]. **means** [DKB23, HRTSS⁺20]. **measure** [AA20]. **Mechanical** [SL20, AQRA⁺23, AAe20, GPEK⁺20, HKSW20, MMK⁺20, MLX⁺24, MMAZ⁺23, PWX⁺20, PGP⁺21, PSA⁺23, SPSH20]. **mechanics** [BRNB21, CLTMd⁺23, DC22b, FDK22, KGD⁺21, TCS⁺21a, VT24]. **mechanics/molecular** [CLTMd⁺23, FDK22]. **Mechanism** [Ban20, CWZD20, WLZM20, ZZ23b, ABZ20b, BAM⁺24, CJHW21, CD20,

CSP20, CRT⁺²¹, DSS⁺²⁴, DOT22, GPM21b, HRTSS⁺²⁰, JWS⁺²⁴, KZJ21, KR23, KLC⁺²⁴, KSS21b, LRqG⁺²², LBH⁺²², MNH21, MIP⁺²², NMMC21, NST⁺²⁰, PPSP20, PM21, RPA⁺²⁴, SVDS21, SMB⁺²³, SKGG23, SCZ⁺²¹, SLML24, YC23]. **mechanism-enabled** [LBH⁺²²]. **Mechanisms** [CGMRVBAI22, WW24, BCN22, ČNF23, LA20, LEP⁺²¹, MNZGO⁺²⁰, NYM22, ONA⁺²⁰, PC21, SWF⁺²⁰, SWM^{+20b}, ZLLL22]. **Mechanistic** [AMM22, BXY⁺²⁴, HCY⁺²², JFZ⁺²⁰, KZJ22, PPRS22, TYZ20, ZMH⁺²¹, ARA22, JAP⁺²⁴, LGJF22]. **mechanistically** [KCF⁺²⁰]. **mediate** [XIV⁺²⁴]. **mediated** [JGSA22, SKGG23, TYZ20]. **medicinal** [BBB⁺²³, TCS^{+21a}]. **medium** [BSS⁺²², GH22b, GH23, LSP23, LRKD23, PDC23, YC20]. **medium-resolution** [LSP23]. **melting** [CST23]. **melts** [WKD⁺²¹]. **membered** [DSB23, KZJ22, LLJ⁺²⁴]. **Membership** [GJMPB⁺²⁰]. **Membrane** [BWM20, FMFG20, HHL⁺²⁰, KCF⁺²⁰, VDK⁺²⁰, CX21b, IBL20, NLC23, ZSD⁺²⁰]. **Membrane-Integrated** [VDK⁺²⁰]. **Membranes** [PT20, AAID22, CBB⁺²¹, MSA22a, WRBT21]. **mer** [HHL⁺²⁰, LGD⁺²⁰]. **mercaptapurine** [NST⁺²⁰]. **mercury** [LGD⁺²⁰, MDO⁺²⁰]. **Merocyanine** [TMO⁺²¹]. **mesh** [RCC21]. **mesophilic** [NYM22]. **meta** [BMT⁺²¹, NG20]. **meta-generalized** [BMT⁺²¹]. **meta-generalized-gradient** [NG20]. **metabolism** [DSS⁺²⁴]. **Metadynamics** [Tik23, KN21, KSRB⁺²¹, LL21a, NN20, PPSP20, TM20]. **Metal** [HHL⁺²⁰, PWW20, AR20, AS23, BKM21, DRBT24, DGM22, DOT22, ENR⁺²⁴, EK20b, FBM⁺²³, HRTSS⁺²⁰, IK21, JMV21, KMR⁺²⁴, MLM⁺²⁴, MAM21, MAI22, MYYS24, MCD22, NBE⁺²³, OM23, OSM20, PTP23, PDGD23, PGDD24, PSM⁺²⁰, POPGS22, SKY24, TYZ20, WP20, YFS20, YMSS23, YSMS24, ZBH⁺²³, dBCdL20, Ari24]. **metal-ammine** [MLM⁺²⁴]. **metal-containing** [ENR⁺²⁴]. **metal-dinitrogen** [DGM22]. **metal-doped** [DOT22]. **metal-free** [TYZ20]. **metal-involving** [ZBH⁺²³]. **metal-ligand** [BKM21]. **metal-organic** [HRTSS⁺²⁰, MAM21, WP20]. **metal-to-ligand** [IK21]. **Metal-Tren** [Ari24]. **metal/** [AR20]. **metallic** [CBF⁺²⁰]. **metallo** [KGD⁺²¹]. **metallo-** [KGD⁺²¹]. **metallocenes** [HSG21]. **metallofullerenes** [DA22]. **metallomimetics** [SLML24]. **metals** [PTP23, VV20b, WW24]. **metastability** [SMH21]. **methacrylate** [MSA22a]. **methane** [DZL⁺²⁰, IMT⁺²¹]. **methanol** [DHN⁺²¹, RPD^{+20a}, SSM21]. **Method** [QB20, AD23, AKN⁺²⁰, ABTM22, AYO20, AiIS⁺²¹, BBK⁺²¹, CK22, DWSX20, Dor20, EK20a, EVKL21, Fed22, Fed24, FBP⁺²², HKFT21, HGR⁺²⁴, HTFY21, IYI⁺²⁰, IN23a, IW24, JGM21, KWX23, LWF⁺²², LRqG⁺²², LC22, MMK⁺²⁰, MA23a, MA23b, MT20b, MSS20, NAN⁺²³, PDL⁺²¹, PSMPB21, RSHG23, SS20, SDH23, SKKK20, SHH^{+23b}, SHH^{+23a}, TTH^{+21a}, WKG⁺²³, XZC⁺²⁴, YLZ⁺²⁰, YAO20, ZK21, ZLLL22]. **method-based** [ZLLL22]. **Methods** [AWID⁺²⁰, KUNT20, PAS⁺²⁰, SK20, ASW20, BPT⁺²³, BSB⁺²⁴, BSF20, BF22, CTPJH22, FB21, GUCCR20, IWN24, KRSD⁺²³, KB22, KBK⁺²⁴, NBE⁺²³, OM22, PW20, PB20, RLHG⁺²³, RvWH23, SW21, SYS⁺²¹, SM22a, SC22, Sts20, SHH^{+23b}, SHH^{+23a}, TZS⁺²²]. **methotrexate** [PRH20].

methotrexate-camptothecin [PRH20]. **methoxyethyl** [MSA22a]. **methoxyphenol** [KLC⁺24]. **methyl** [CCZ23, OAN⁺23, PGP⁺23, SKGG23]. **methylene** [ERVN24]. **methylide** [SVTK⁺22]. **Metropolis** [EG20]. **Mg** [SM22b, DSC20, GP21, JRS20, ZRSST20, ZDBZ20]. **MgCl** [AMM22]. **MgO** [DA22]. **MH** [WTST24a]. **micellization** [ZK21]. **micro** [VHS⁺24]. **micro-kinetic** [VHS⁺24]. **microhydrated** [GJL21]. **microkinetic** [CJHW21, SC23]. **Microscale** [HZG⁺20]. **Microscopic** [PT20]. **microscopy** [Yos24]. **Microsecond** [SSPK24]. **microsolvated** [OM22]. **microsolvation** [STR20]. **MIDAS** [GJMPVR⁺20]. **midbond** [MEKH22]. **milder** [GM22]. **mimetic** [HTFY21]. **minerals** [RCD⁺24]. **Minimal** [HHL⁺20, JGGPN21]. **minimize** [AiIS⁺21]. **minimizing** [YBS⁺20]. **minimum** [DC22a, RH21, SDH23]. **mismatch** [CR24]. **Mixed** [CDCT21, WTST24a]. **Mixed-solvent** [CDCT21]. **mixture** [NS22]. **MkVsites** [LKM20]. **ML** [TTK23]. **MLLPA** [WRBT21]. **MM** [ABNG22, BBC20, GH22a, LRqG⁺22, LSCK23, Mar21, PCI23, SSS⁺20a, SHH⁺23b]. **MM-PBSA** [SHH⁺23b]. **Mn** [TAB⁺24]. **MNDO** [FCB23]. **MNDO-MD** [FCB23]. **Mo** [MAM21]. **Mo-Oxo** [MAM21]. **mobilities** [LHC⁺21]. **MoBioTools** [CLTMd⁺23]. **MOCASSIN** [EG20]. **mode** [BEKM24, FDK22, FAK24, San21, SH23].

Model
 [GCL⁺20, HRT⁺20, LGM20, MT20a, SSS⁺20a, BW22a, BPDG21, BK24, CC22, CX21b, CQSG20, DKB23, GSH23, Gie21, HKSW20, HPG20, IN23b, IK21, IL24, KWYN23, KdILC22, KPKS23, LC22, MDO⁺20, MT19, MGCM21, NGD22, PDL24, RPD⁺20a, SWF⁺20, SWM⁺20b, SSO⁺20, SHH⁺23a, TLD⁺22, UB20, VL22, VAL20, VFCG20, WCY⁺24, WKL22, XAD20].

model-compounds [BW22a]. **model/energy** [MGCM21]. **modeler** [SKS21]. **Modeling** [AWID⁺20, BLP20, BS23, CMG⁺24, FVSS20, GNK⁺23, KDLP21, KB22, LJ20, LWLC21, LDT⁺22, PAF⁺20, RCD⁺24, SHM⁺20, ZOD⁺22, BHR⁺21, CFOMCB⁺22, COK22, GWN21, GUCCR20, KGTL21, Kos22, LLS22a, LGD⁺20, LL21b, LL22, MGB⁺22, MZ21, MSA22b, NDK24, PJJL23, PSG21, SSFS22b]. **models** [AVM21, BK22, BSR22, BP22, CCHS23, CTBB20, DGS24, HPM⁺21, JGGPN21, KK23, KOD21, KTBS23, LGJF22, LBH⁺22, LMPT21, MP24, MK22a, PLP⁺20, PSW⁺24, PMT⁺22, PCI23, SKL23, SJA24, UB20, VHS⁺24, WP20]. **modes** [CBF⁺20, dBCdL20].

Modification [AWID⁺20, Ban20]. **Modified** [SG20, DOT22, XAD20, ZHG⁺24]. **Modifying** [PFPD21]. **modular** [RBM⁺23]. **Modulation** [ZSD⁺20]. **module** [WRBT21, WLSC23a]. **MOF** [ZHG⁺24, FP23]. **moiety** [KPTT21]. **Molecular** [ARR22b, BR23, BCN22, CA22, FBM⁺23, FMFG20, GJMPB⁺20, GGK20, GCL⁺20, JRS20, KR23, KUNT20, MPOC21, MSA22a, NLC23, WCT⁺23, YXGZ20, Zac20, AV20, ARR22a, AD23, AKGD24, AKN⁺20, AAL21, AÅFJ21, AiIS⁺21, AR24, AS20, ALA⁺22, AMF⁺20, BUNO22b, BdLC21, BRNB21, BAO⁺20, BSB⁺24, BTL24, BOPJ⁺21a, BP22, CFOMCB⁺22, CLTMd⁺23, CDCT21, CX23, Che23, CSP20, CMD⁺22, CST23, DGS24, DO20, DHN⁺21, DHD21, EVKL21, Fed22, Fed24, FDK22, FNY21, Gao20,

GJMPVR⁺²⁰, GK24, GG22, GSJ⁺²³, HS23, HGF20, HPM⁺²¹, IAS⁺²⁴, JKK⁺²¹, KZJ21, KG23, KK23, KI24, KLP⁺²², KTBS23, KPHV23, KS24, KGD⁺²¹, LL21a, LKM20, LHH⁺²¹, LKK⁺²³, LKT21, LCLB24, LEP⁺²¹, LAM⁺²³, MP24, MN20, MKK⁺²², MGB⁺²², MSA⁺²⁴, MK22a, MAP⁺²⁰, NAN⁺²³, NI22, NGD22, NN20, NP23, OSHT20, PBM21, PDL⁺²¹].

molecular

[POvG21, PPP21, PL22, PSB⁺²², PM21, QLC⁺²⁰, RKC21, RDK⁺²², RGGD21, RPD^{+20a}, RDB23, RDS⁺²⁰, SFS24, SPSH20, SIW21, SYS⁺²¹, SAZ⁺²³, SCvW22, SKL23, Shi22, SY21, SWLC22, SMB⁺²³, SKKK20, SZL23, SCCZ21, TWT⁺²², TPB22, TCS^{+21a}, TSR21, UKBD23, VKSS24, WTST24a, WFBB22, WK21, WKL22, WKD⁺²¹, YGG⁺²³, Yos24, YC23, YrYqLhC23, YMM⁺²⁴, ZK21, ZG21, ZWR22, ZZ23a, ZFRM20, KZJ22].

molecular-dynamics [UKBD23]. **molecular-orbital** [KK23].

molecular-wide [BdLC21]. **molecule** [AK20, BBBP⁺²³, GFRNC21, KDMM24, KFTB20b, MC24, Mon24, Ore24, SKL23, TANC23, YIO20, ZK23].

Molecules [LPP20, AFR^{+24a}, APS20, AG21, AZKM22, AA20, BMA⁺²⁴, BA24, BGS⁺²⁰, CKH23, CdSB⁺²¹, FB20, GGK20, GP21, HTTT23, Jab22b, KWX23, KZOV23, KPR23, KdILC22, KPHV23, KYM20, LPF⁺²³, LGM20, LGM22, LK22, LT23, LYX⁺²², LJW⁺²³, MPP23, MC23, MLP22, MB21, NTK21, PFP⁺²¹, PGH24, SRB21, Sch22a, Sch22b, SCC⁺²², SSO⁺²⁰, SHH^{+23b}, SLML24, TIK21, TMO⁺²¹, TSR21, VCL20, WLWR22].

molecules-in-molecules [TSR21]. **Møller** [CSGVF⁺²⁰, FKT21, Sán20].

Møller-Plesset [CSGVF⁺²⁰, Sán20]. **molSimplify** [ENR⁺²⁴]. **MolSpin**

[GNK⁺²³]. **moments** [BSF20, LRKD23]. **Momentum** [FNY21, MR21].

Mono [ZXD20b, ZXD20a, HBM⁺²⁰, MAKZ23]. **mono-** [MAKZ23].

Mono-silicon [ZXD20b, ZXD20a]. **monodentate** [TLS23]. **monolayers**

[LHC⁺²¹, MMAZ⁺²³]. **monomer** [ZLLL22]. **monooxygenase** [HYA⁺²⁰].

Monte [DMD⁺²¹, EG20, GGK20, GNL⁺²², KCGK20, KEK23, PFSC20,

TIK21, TMO⁺²¹, ZKJ⁺²³]. **Monte-Carlo** [GNL⁺²²]. **MonteCarbo** [AG21].

MoO [SM22b]. **moon** [HBM⁺²⁰]. **MOPAC** [Gie21]. **MoSDeF** [DMD⁺²¹].

motif [HS23]. **motifs** [HC21, YrYqLhC23]. **motions** [BBSFA22, San21]. **MP**

[ABTM22]. **MP2** [KG23, MEKH22, SW21]. **MP2/CCSD** [KG23].

MPCONF196 [PGH24]. **MPI** [AiIS⁺²¹, RB24]. **MPI-parallelization**

[RB24]. **MRCI** [ZRSST20]. **MSMS** [WK21]. **Mukaiyama** [LLS^{+22b}].

Multi [HREvdK⁺²⁰, AFR^{+24a}, AS23, BBB⁺²³, BMT⁺²¹, CMO⁺²⁴,

PMT⁺²², SY21, VM23]. **multi-decker** [AS23]. **multi-descriptor**

[CMO⁺²⁴]. **multi-parametric** [PMT⁺²²]. **multi-purpose** [BMT⁺²¹].

multi-reference [VM23]. **Multi-scale** [HREvdK⁺²⁰, SY21]. **multi-step**

[AFR^{+24a}]. **multi-use** [BBB⁺²³]. **multicanonical** [BAO⁺²⁰].

multiconfigurational [HRTSS⁺²⁰, TT20]. **multicore** [GJMPVR⁺²⁰].

multideterminant [KRSD⁺²³]. **multidimensional** [BCN22, GWN21].

multifunctionalized [AG21]. **multilayer** [IRB⁺²³]. **multilevel** [SW21].

Multilinear [WSL⁺²⁰]. **Multimolecular** [GP21]. **Multiple**

[SZLD20, MKK⁺²², POvG21, WCT⁺²³, XAD20]. **multiple-time-step**

[POvG21]. **Multipolar** [HRT⁺20, YFH⁺21]. **multipole** [AYO20, AiIS⁺21, MSS20, YAO20]. **multipurpose** [TSZ⁺21]. **multireference** [SD21, UR23]. **Multiscale** [SSFS22b, FLT23, LGD⁺20, LGC21, Mar21]. **mussel** [MSA22a]. **mussel-inspired** [MSA22a]. **mutant** [BK22, CSP20]. **mutation** [SSPK24]. **mutations** [HB21, WCY⁺24]. **Mutual** [SKT24]. **Mycobacterium** [RDK⁺22].

N [ZHG⁺24, ZDBZ20, ARR22b, BSS⁺22, DZL⁺20, GKA⁺23b, JGSA22, MKSS20, PAS⁺20, RC22, XLW⁺22, TTK23]. **N-co-doped** [DZL⁺20]. **N-heterocycles** [BSS⁺22]. **N-heterocyclic** [JGSA22]. **N-Terminal** [MKSS20]. **NADH** [CFOMCB⁺22]. **NADH-fumarate** [CFOMCB⁺22]. **NADP** [CWZD20]. **NADPH** [CWZD20]. **named** [SS20]. **nano** [FDD⁺23]. **nano-hoops** [FDD⁺23]. **nanobelts** [AS21]. **nanoclusters** [GAG20, MK22b]. **nanocrystals** [KPR23, Mil21]. **nanodiamonds** [KPDB22, KWB24]. **nanometer** [NAAP21]. **nanoparticle** [LBH⁺22]. **nanoparticles** [BA22, IL24]. **nanopores** [YC20]. **nanoreactor** [FP23]. **nanoribbons** [SPT21]. **nanoring** [YLZ⁺22]. **nanoscale** [SG20]. **nanoscopic** [CR24]. **NanoShaper** [WK21]. **nanostructures** [Che23]. **nanotube** [APS20, CTBB20]. **Nanotubes** [DBE20, BW22a, CBF⁺20, VCL20]. **Naphthalene** [NRH⁺20]. **naphthyridine** [WCD⁺23]. **naphthadithiophene** [BMA⁺24]. **naphthadithiophene-based** [BMA⁺24]. **Natural** [KL20, CB20, GRBN21, MH20, PW20, RPA⁺24, Sch22b, SD21]. **Nature** [MVP⁺20, PDC23, WG21, BRNB21, BPDG21, JX24, FDD⁺23, HSG21, Jab22b, KLC⁺24, KSP21, MC23, MP23, NTK21, Wan21a, Wan21b, dARW⁺23]. **NaY** [NS22]. **NbGe** [TT20]. **NBO** [LGJF22]. **NbX** [ABAQ⁺23]. **NCF** [OE20]. **NE-RDFE** [MPP23]. **near** [IRB⁺23]. **needs** [NGD22]. **negative** [TAC⁺23]. **neighbor** [GKO⁺22]. **neon** [LZW⁺23]. **neopentane** [NS22]. **NeRF** [ABTM22]. **Nernst** [CX21b]. **net** [ÖLP⁺20]. **net-charge** [ÖLP⁺20]. **Network** [BSL20, KRW⁺24, KOD21, MZ21, MLP22, NGD22, RTB23, SSM21, TIK21, WCY⁺24]. **networks** [SKY24, VFCG20]. **neural** [KRW⁺24, MZ21, MLP22, NGD22, SKY24, TIK21]. **neuraminidase** [SSPK24]. **neuroglobin** [FDK22]. **Neutral** [LL21a, BGS⁺20, KPKS23, MCP23, MP23]. **Neutralizing** [KUNT20]. **never** [SVR⁺24]. **NEVPT2** [CS20]. **Newton** [MT20b]. **Next** [AMF⁺20, LYX⁺22]. **Next-generation** [AMF⁺20]. **Ng** [APR21]. **NgX** [APR21]. **NH** [OE20, XZW⁺21, HS23, SLR⁺20]. **NHCs** [DSB23]. **Ni** [LXP⁺22, SM22b, BXY⁺24, MYYS24, PTP23, SS24, ZHG⁺24]. **Ni-catalyzed** [BXY⁺24]. **Ni-MOF-74** [ZHG⁺24]. **NIAS** [FPMD23]. **NIAS-Server** [FPMD23]. **nickel** [DSK21, LLKS23, ZZG⁺21]. **nickel-nickel** [LLKS23]. **nicotinic** [BRNB21]. **nitrate** [YC20]. **Nitreones** [PAS⁺20]. **nitride** [NDK24]. **nitriolotriacetate** [CL23]. **nitrite** [YC20]. **nitroalkenes** [KZJ22]. **nitrobenzaldehyde** [VM23]. **nitrocellulose** [ZLLL22]. **nitrogen** [JMV21, XZZ⁺20]. **nitrogen-rich** [JMV21]. **nitrogenase** [GKA⁺23b, WS21].

nitroimidazole [CFOMCB⁺22]. **nitronates** [KZJ22]. **nitrone** [BAM⁺24].
nitroprop [SMB⁺23]. **nitrosyl** [KK23]. **nitrous** [KZJ21]. **nitroxide**
 [MC23]. **NLi** [SKKG22]. **NMR** [Ben22, CMG⁺24, FBP⁺22, KWX23, LL22,
 MPOC21, MPV22, MCD22, Sai23, TTDT20]. **NMR-data-assisted** [LL22].
NN [LPP20]. **NO** [OKI⁺21]. **Noble** [YSMS24, APR21, MSYS23, YMSS23].
NOCV [DGM22, GM22, GKA⁺23b, SBB⁺22, SM23]. **Noggin** [CM20b].
Non [GAP21, KE23b, BdLC21, LGJF22, MP23, SKT24, TAC⁺23, VV21].
non-aqueous [VV21]. **non-bonding** [MP23]. **non-classical** [BdLC21].
non-covalent [SKT24]. **non-iterative** [VV21]. **non-negative** [TAC⁺23].
Non-nuclear [KE23b]. **non-thermal** [LGJF22]. **nonadiabatic** [SWM⁺20b].
nonaqueous [RPD⁺20a, SJA24]. **noncovalent**
 [BW22a, CSWW20, CTBB20, OE20, OM23, RMJ21, Sch22b, YW20].
nonelectrostatic [VL22]. **nonequilibrium** [MPP23]. **nonfullerene**
 [TANC23]. **Noniterative** [HFPS20]. **Nonlinear**
 [BSR22, RMBSPJSG24, SNN⁺21]. **nonlocal** [RMJ21, TV22, YW20].
Nonredundant [XZ20]. **Nonrigid** [Bal20b]. **nonuniform** [YLZ⁺20].
norbornadiene [Dor20]. **norbornene** [MCD22]. **norcarane** [MNH21].
Normal [San21]. **Normal-mode** [San21]. **norovirus** [LSC⁺23]. **Novel**
 [SEBE21, VT24, LHC⁺21, PPP21, RDK⁺22, RD24, SS20, VWP⁺22]. **ново**
 [PMT⁺22, TIK21]. **NS5B** [MPuS⁺20]. **NSP15** [SLMA21]. **nuclear**
 [IN23b, KE23b, LCC⁺21, LL21b, VCL20].
nuclear-magnetic-resonance-assisted [LL21b]. **nucleation** [KEK23].
nucleobases [BVGB23, CTBB20]. **nucleophilic** [CRT⁺21]. **nucleotide**
 [XZX⁺22]. **Nudged** [MA23b, MA23a, ZLLL22]. **Number** [VHS⁺24, MT20b].
numbers [ASW20, SD21]. **numbers-based** [SD21]. **numerical**
 [CX21b, DWZ22, GWN21, Pan23].

O [GJL21, KPTT21, LZW⁺23, TTK23, AWK⁺23, DK23, IAF⁺24, KPTT21,
 MC23, MCP23, MBBU23, SGSB23, SWF⁺20, SWM⁺20b, SVTK⁺22, TYZ20].
O-compounds [MCP23]. **O-H** [KPTT21]. **Obelin** [GOY20]. **obtain**
 [dMBdAVdS24, FNY21]. **obtained** [UKBD23]. **OC** [HS23]. **occupation**
 [ASW20, Sch22a, SD21]. **occupied** [KPHV23]. **OCOH** [dCVARN20].
octahedra [PGDD24, PDL24]. **octamer** [Bal20b]. **octanol** [SHH⁺23b].
OCTMCCO [LZW⁺23]. **O =** [ARR22b]. **off** [LK22]. **off-center** [LK22].
offs [WKL22]. **OLEDs** [ZWL24b]. **oligonucleotides** [KZOV23]. **Omicron**
 [KLZ⁺23]. **on-surface** [LHG⁺23]. **On-the-fly** [APP24, OSHT20, RBM⁺23].
one [BBC⁺21a, SNK24b, WKG⁺23]. **one-electron** [BBC⁺21a]. **one-photon**
 [SNK24b]. **one-step** [WKG⁺23]. **ONIOM** [KWX23]. **online** [WRVP22].
onto [AWK⁺23]. **OO** [SVTK⁺22]. **Open**
 [SM23, AAID22, FR21, HAC⁺23b, IW24, MNBG⁺21, PSGL21, RBM⁺23].
open-shell [IW24]. **open-source**
 [AAID22, FR21, HAC⁺23b, MNBG⁺21, PSGL21, RBM⁺23]. **Opening**
 [VDK⁺20]. **OpenMM** [BPT⁺23]. **operators** [BBC⁺21a, CTPJH22]. **OPLS**
 [ZWY⁺22]. **OPLS-AA** [ZWY⁺22]. **oppositely** [HPG20]. **optical**

[AQRA⁺23, BA22, BSR22, JS21, JMV21, LM24, LRKD23, PSA⁺23, RMBSPJSG24, STB⁺20, TAB⁺24, Tou21]. **optically** [TIK21]. **Optimal** [WZZ⁺20, YBS⁺20, SCvW22]. **Optimization** [LPP20, MFS22, SSDL⁺23, AZKM22, CTPJH22, MLC⁺23, MZ21, MB21, MT20b, NAAP21, PDGD22, PMT⁺22, SM20, SHH⁺23a, TV22]. **optimizations** [GSD⁺22, LSCK23, MMK⁺20]. **Optimized** [GH22a]. **optimizing** [RDB23]. **Opto** [AQIS⁺24, BMA⁺24]. **Opto-electronic** [AQIS⁺24, BMA⁺24]. **Optoelectronic** [dCB23, AQMM⁺23, ZGZ⁺20]. **orbit** [PHS⁺20, POPGS22]. **Orbital** [AD20, BBK20, KUNT20, LCC⁺21, SCKH21, AKN⁺20, ASW20, CB20, Fed22, Fed24, GRBN21, HTTT23, HCS⁺20, KK23, KPHV23, MSA⁺24, NAN⁺23, NEG⁺20, PDL24, PW20, Sch22b, SD21, TWT⁺22, TSH⁺23, VKSS24]. **orbital-based** [TWT⁺22]. **orbitals** [BTSB22, FV20, KL20, MH20]. **order** [CSGVF⁺20, DTA21, EVKL21, FKT21, FYIO23, GX20, HD21, QLW⁺22b, Sán20, YW20]. **ordering** [PDL24]. **Organic** [LPP20, AFR⁺24a, AZKM22, CCZ23, FB20, GGK20, HRTSS⁺20, KGS⁺21, KS21, KPHV23, LPF⁺23, LCP24, LMPT21, MAM21, MLP22, NI22, SC22, SZP⁺20, TANC23, TIK21, TSH⁺23, WP20, ZGZ⁺20]. **organic-inorganic** [KGS⁺21, SZP⁺20]. **organo** [SKY24]. **organo-transition** [SKY24]. **organocatalysts** [FP22]. **organophosphorus** [AR24, PDP⁺24, TYZ20]. **orientation** [KPR23, RH21, SCC⁺22]. **oriented** [GZFSM21, NSRK21]. **Origin** [EK20b, MIK⁺23, PP23, RMS⁺23, DMTR22]. **Origins** [JFZ⁺20, BXY⁺24, TANC23]. **ortho** [VM23]. **ortho-nitrobenzaldehyde** [VM23]. **orthogonal** [CB20]. **oscillators** [BS23]. **Other** [FMFG20, TAC⁺23]. **outcome** [DGS24]. **overlap** [BK24, CTPJH22]. **Overlapping** [RTB23]. **Overreact** [SC23]. **Oversampling** [NNT⁺20]. **oxa** [NMMC21]. **oxa-Diels** [NMMC21]. **Oxidation** [CWZD20, KM22, LJW⁺23, MKB⁺21, PM21]. **oxidative** [IMT⁺21, KPDB22]. **oxide** [AMM22, MK22b, RMS⁺23, RCD⁺24, SGRN24, TYZ20]. **oxides** [RZS⁺23]. **Oxidized** [CWZD20]. **oxidozirconium** [CMD⁺22]. **oxindoles** [SKGG23]. **oxo** [MIP⁺22, MAM21]. **OxoMn** [MNH21]. **Oxygen** [GOY20, HL20, KZ24, NAAP21, SGRN24, SaATR24, WW24]. **oxygen** [SaATR24]. **oxygen-centered** [KZ24]. **oxygen-oxygen** [HL20]. **oxygen-preadsorbed** [WW24]. **oxynitride** [HM21].

P [SGSB23, ARA22, CMG⁺24, FBP⁺22, HYA⁺20, IW23, SSSA23, SHHH22]. **P-NMR** [CMG⁺24]. **p-phenylenediamine** [ARA22]. **P-surface** [IW23]. **package** [AME⁺21, BPT⁺23, CKH23, HAC⁺23b, KZOV23, KYM20, LHH⁺21, MWK⁺20, MY24, SSDL⁺23, VWFR21, YWGY22]. **packet** [SWM⁺20b]. **Paddlewheel** [AD20]. **Pair** [SLR⁺20, GRBN21, HPG20, Ore24, PW20, QLC⁺20, dSSRVdM24, ZS22]. **pairs** [FP22, MC24, TTDT20]. **pairwise** [KRW⁺24, YBS⁺20]. **para** [SW21]. **para-substituted** [SW21]. **ParaCopasi** [YWGY22]. **parallel** [ABTM22,

BBK⁺²¹, CP23, GVJ⁺²², JKK⁺²¹, JKS23, SSDL⁺²³, WMZJ20, YWGY22].
parallelization [NN20, RB24, YLZ⁺²⁰]. **parallelized** [AiIS⁺²¹].
paramagnetism [GSSG24]. **parameter** [POPGS22, RB22].
parameterization [OC23]. **Parameterizing** [KOD21]. **parameters**
 [BTL24, BK24, DTA21, GH22a, KDLP21, LKM20, LBH⁺²², MH22, PNT⁺²²].
parametric [PMT⁺²²]. **parametrization** [GKO⁺²², KYM20]. **part**
 [MR21, MPR22, RLHG⁺²³]. **partial** [LK22, MM24]. **particle**
 [CN21, WKD⁺²¹]. **particle-field** [WKD⁺²¹]. **particles** [LSC⁺²³].
partition [AYO20, CSGVF⁺²⁰, LC22, SHH^{+23b}]. **Partitions** [TLD⁺²²].
Parzen [AZKM22]. **PASSerRank** [TXJT23]. **Path**
 [SZLD20, Shi22, AKR21, GSD⁺²², RH21, TAB⁺²⁴]. **paths**
 [ETT21b, MA23b, SDH23]. **pathway** [DSB23, HL20, PPRS22, XZC⁺²⁴].
pathways [AST24, BBC20, CG20, DWSX20]. **pattern** [XDZ23]. **patterns**
 [HS22, KLZ⁺²³]. **Pb** [LXP⁺²², WTST24a]. **PbI** [XZW⁺²¹]. **PBSA**
 [SHH^{+23b}, SHH^{+23a}]. **PCM** [CC22]. **Pd** [ABZ20b, PTP23, SS24].
Pd-PEPPSI [ABZ20b]. **PDB** [RB22]. **PDB-to-parameter** [RB22]. **PdBe**
 [Tze21]. **PEACH** [ZK21]. **PEB8** [BR23]. **PEC4** [BR23]. **PEC8** [BR23].
penicillin [CD20]. **pentacoordinate** [FDK22]. **pentaerythritol** [BR23].
pentahalides [PT21]. **Pep** [SKS21]. **PepPro** [XZ20]. **PEPPSI** [ABZ20b].
peptidase [CD20]. **Peptide**
 [XZ20, EIT⁺²¹, GG22, KZOV23, SKS21, SSS^{+20b}, UAC⁺²³].
peptide-based [KZOV23]. **Peptide-Protein** [XZ20]. **peptides** [PRIP24].
per- [MHA⁺²³]. **perfluorinated** [FDD⁺²³]. **perfluoroalkyl** [MVV22].
perform [CKH23, MY24]. **Performance**
 [BBK20, GSH23, NRH⁺²⁰, PB20, BLB20, LKM20, MH22, MKK⁺²²,
 OKI⁺²¹, SFS24, dASRHB21, SS24, TTK23]. **performed** [MAM21].
Performing [Zac20, FYIO23]. **period** [LB21, LB22]. **Periodic**
 [SDK20, HAC^{+23b}, PKT21, PSMPB21, SZP⁺²⁰, YAO20]. **Periselectivity**
 [SHH⁺²⁴]. **permeability** [ZSD⁺²⁰]. **permutation** [FYIO23].
Permutationally [OKK22]. **perovskite**
 [AQRA⁺²³, LM24, SZP⁺²⁰, XZW⁺²¹]. **perovskites**
 [AQMM⁺²³, ABAQ⁺²³, KGS⁺²¹, PGDD24, PDL24, dARW⁺²³]. **peroxide**
 [CL23, DHN⁺²¹]. **peroxides** [MC23, WKG⁺²³]. **peroxy** [WKG⁺²³].
persistent [BPDG21]. **perspective**
 [AVM21, BBL⁺²², DF22, LKAT22, LT23, NI22, PPSP20, SWM^{+20b}, SCC⁺²²].
persulfate [ARA22]. **Perturbation**
 [NNT⁺²⁰, AAe20, FKT21, GX20, MH20, NTK21, OE20, Sán20, YBS⁺²⁰].
perturbations [PKT21]. **perturbed** [PDGD23]. **pesticide** [BTL24]. **PFAS**
 [MPV22]. **Pfizer** [GLC⁺²²]. **PH** [PT20, CR24, SSS^{+20a}, WdGG24].
pH-consistent [CR24]. **pharma** [IRB⁺²³]. **pharmacophore**
 [KDP⁺²², MLG^{+21b}]. **pharmacophore-based** [MLG^{+21b}]. **PharmRF**
 [KDP⁺²²]. **Phase**
 [HFPS20, VFCG20, AZKM22, BPT⁺²³, CM20a, DC22b, EK20c, IMT⁺²¹,
 LWF⁺²², OM23, SW21, SGSB23, SNK24b, WRBT21, YW20].

phase-specific [WRBT21]. **Phasepy** [CM20a]. **phenanthroline** [SGGG22].
phenomenological [DWSX20]. **phenyl** [AS20, THLC⁺23].
phenylacetohydroxamic [CMD⁺22]. **phenylenediamine**
 [ARA22, LDT⁺22]. **pheophytin** [Tou21]. **pHLIP** [FM21]. **phonon** [SS24].
Phonons [DBE20]. **phosphate** [DPSG20, HUUO23, SGRN24, SGGG22].
phosphine [SGRN24]. **phosphorane** [STB⁺20]. **phosphocholine** [ZK21].
phosphodiester [GP21]. **phosphoglucose** [DPSG20]. **phosphorescent**
 [WYC⁺24]. **phosphorus** [ASL⁺20, HM21]. **phosphorus-based** [ZS22].
phosphoryl [SGRN24]. **photo** [CCPR24, KFTB20b]. **photo-induced**
 [CCPR24]. **photo-switchable** [KFTB20b]. **photoacidity** [GSH23].
Photocatalytic [BWS20]. **photochemical** [CG20]. **Photochemistry**
 [FCPG20]. **Photodissociation** [dSSRVdM24]. **photodynamic**
 [ASL⁺20, DART21, RPA⁺24, DMTR22]. **photoionization** [AAL21].
Photoisomerization [YXGZ20]. **photon** [SNK24b]. **photooxidation**
 [KDKS21]. **Photophysical** [DART21, WYC⁺24]. **Photophysics** [BVGB23].
photoproperties [TANC23]. **Photoprotein** [GOY20]. **photoresponsive**
 [YLZ⁺22]. **photosensitizers** [ASL⁺20, DART21, RPA⁺24].
photosensitizing [HREvdK⁺20]. **photoswitches** [HPM⁺21]. **photovoltaic**
 [KGS⁺21]. **phthalocyanines** [DART21]. **Physical**
 [PFP⁺21, YJZ⁺22, BMT⁺21, Jab22b, RMS⁺23, TANC23]. **physico**
 [CSG⁺21]. **physico-chemical** [CSG⁺21]. **physicochemical** [KZP22].
physisorption [RC22]. **PI** [AMM22]. **Picture**
 [QLW⁺22b, GCP22, JGGPN21]. **Picture-word** [QLW⁺22b]. **pincer**
 [DSK21, YYS20]. **pincer-nickel** [DSK21]. **pistol** [JRS20]. **pK** [PWW20].
planar [DC22a, YrYqLhC23]. **planarization** [KK22c]. **Planck** [CX21b].
plane [MN20]. **planewave** [SM20]. **plasma** [LGJF22]. **Plasticity**
 [AD20, SSPK24]. **platform** [BBB⁺23, CSG⁺21, PSGL21, ZK23].
platform-independent [CSG⁺21]. **platinum**
 [HBM⁺20, NAAP21, WYC⁺24]. **play** [FM21, KE23b]. **Plesset**
 [FKT21, CSGVF⁺20, Sán20]. **plugin** [EK20a]. **PMe** [PTP23]. **pnicogen**
 [KS24]. **Pnictogen** [AR24]. **pockets** [XZX⁺22]. **Point**
 [MXM20, BSF20, CST23, MH22, PP23, PKT21, TTK23]. **points** [DTA21].
Poisson
 [BSB⁺24, CX21b, NSRK21, RCC21, SCvW22, UYJ⁺24, WK21, XAD20].
polarity [DK23]. **polarizabilities** [LRKD23]. **polarizability** [OKK22].
Polarizable [HRT⁺20, LJ20, UB20, ALA⁺22, GP21, KLP⁺22, KYM20,
 KGD⁺21, LRqG⁺22, ODL20, WLWR22]. **Polarization**
 [Fed22, LB21, LB22, LLZ⁺23, MAM21, SKKK20, SSO⁺20]. **polarized**
 [NBE⁺23, PDGD23]. **Poltype** [WLWR22]. **poly** [LDT⁺22, MSA22a].
polyacenes [MG24]. **polyacethylene** [BSR22]. **polyalcohol** [KSRB⁺21].
polyatomic [SSO⁺20]. **polyazaheterocycle** [MIP⁺22]. **polybase** [HLV⁺24].
polychromism [RCD⁺24]. **polycyclic** [GAP21]. **polydiacetylene** [NLC23].
polyenes [FCB23]. **Polyethyleneimine** [BAC20, MT21, TPB22].
Polyethylenimine [MT20a, MT19]. **polyfluoroalkyl** [MHA⁺23]. **polymer**

[AFR⁺24a, Che23, WKD⁺21]. **polymer-grafted** [Che23]. **polymeric** [AÄFJ21]. **polymerization** [ARA22, MLB⁺23, MYYS24, OSM20, XZZ⁺20]. **polymers** [LDT⁺22, MMK⁺20, VCL20]. **polymorphism** [CX23, RMS⁺23]. **polymorphs** [KGG21]. **polynomial** [OKK22]. **polyolefin** [KDKS21]. **polypeptoids** [RR22]. **polysulfides** [SC22]. **population** [BA24, LBH⁺22]. **porE** [TS21]. **porosities** [TS21]. **porous** [GGK20, SGT⁺20]. **porphyrin** [MNH21]. **porphyrinic** [KBHG23]. **Portably** [WMZJ20]. **Poses** [SZLD20]. **position** [FNY21, RH21]. **position-dependent** [FNY21]. **Positron** [SSO⁺20]. **possibilities** [LLKS23]. **possible** [ASL⁺20, DART21, SLMA21, WKG⁺23]. **posteriori** [BMT23, WFLZ23]. **potent** [BHR⁺21, CBK⁺24, ZOD⁺22]. **Potential** [KFTB20b, PCB⁺24, APP24, AS20, BBC⁺21a, ERVN24, EK20a, GFRNC21, GP21, HS23, HPM⁺21, KRW⁺24, KM22, KSRB⁺21, Kop22b, KS24, KGD⁺21, MSL⁺20, MK22b, OKI⁺21, PPRS22, RKC21, SDK20, Sts20, SSO⁺20, THH⁺24, Tik23, WTST24a, WRVP22, XLW⁺22, XZC⁺24, YFH⁺21, ZZ23a]. **potential-energy** [MSL⁺20]. **potentials** [BSS⁺22, BBC⁺21a, Cha24, GWN21, LT23, MLB⁺23, MAM⁺23, MLP22, PSW⁺24, RLHG⁺23, SM22b, SG20, TTK23, ZFRM20]. **ppdx** [COK22]. **Pr** [SLML24]. **preadsorbed** [WW24]. **precatalyst** [ABZ20b]. **precision** [XLW⁺22]. **precomputed** [BTC24]. **preconditioning** [RH21]. **precursor** [BVC⁺23]. **precursors** [GM22]. **predefined** [BBSFA22]. **predict** [BA24, Ben22, PDP⁺24]. **predictability** [NGD22]. **Predicted** [CLS⁺20, LWF⁺22]. **Predicting** [APS20, BF22, DRBT24, HBT⁺20, KLC⁺24, MYYS24, QLW⁺22b, WCY⁺24, HLV⁺24, MPuS⁺20, MPV22, NTK21, PB20, SCZ⁺21]. **Prediction** [BUNO22b, CLS⁺20, DHD21, GOY20, LPP20, NMFI21, PWW20, SEZ20, SB20, SHHH22, SHH⁺23b, TXJT23, YFS20, ABZ20b, AAe20, AS23, DPY⁺22, Dor20, GSSG24, KZP22, KSRKS21, LRF⁺21, PWX⁺20, SHH⁺23a, TWT⁺22, UB20, XLW⁺22, YBS⁺20, YGG⁺23, ZHHS21, ZMH⁺21]. **Predictions** [WYC⁺24, DGS24, WCT⁺23]. **predictive** [FB20]. **prefer** [APS20]. **preference** [PFPD21]. **preferences** [DA22]. **Preliminary** [GP21, ZLLL22]. **preparation** [CR24, PBM21, QLC⁺20]. **prepare** [WKG⁺23]. **prepareforleap** [RB22]. **prepper** [KLP⁺22]. **Pressure** [HUUO23, SL20, EK20b, EK20c, GNL⁺22, KGG21]. **Pressure-assisted** [HUUO23]. **pressure-induced** [EK20b, EK20c]. **primary** [ZWY⁺22]. **principle** [LM24]. **Principles** [DBE20, AWK⁺23, BRNB21, DLH⁺23, EK20b, EPT21, KDKS21, KPKS23, PM21, SS24]. **principles-based** [PM21]. **PrNCN** [SLML24]. **PrNCO** [SLML24]. **Probability** [TLD⁺22, RD23]. **probe** [KTBS23, NP23]. **Probing** [GH22a, WG20, Tou21]. **problem** [DWSX20, LBH⁺22]. **problems** [MA23b]. **procedure** [AFR⁺24a]. **Process** [WLZM20, BP22, KK23, MP24, PRH20, SS23, WG20, XZX⁺22, dCRM21]. **processes** [SSFS22b]. **Processing** [GCL⁺20, DWZ22]. **prodrug** [PRH20, PPSP20]. **Producing** [BP22]. **product** [WMZJ20]. **profile** [CSG⁺21]. **profiles** [HBM⁺20, SSS⁺20a]. **profiling** [SEBE21]. **program**

[AKGD24, BK24, Che23, LKK⁺23, MNBG⁺21, PBM21, SWLC22, TSZ⁺21, WFBB22, XSP⁺23]. **Progress** [BGS⁺20]. **projection** [CTPJH22, VCL20]. **projections** [NEG⁺20]. **projector** [DGSB⁺20, NEG⁺20]. **projector-augmented-wave-based** [NEG⁺20]. **projector-based** [DGSB⁺20]. **prolapse** [GH22b, GH23]. **proline** [HB21]. **promenades** [MSL⁺20]. **Promising** [CP23, TAB⁺24]. **promoted** [OSM20]. **promotion** [MGCM21]. **propene** [BR23, DRBT24, LLS⁺22b]. **propensities** [DB23]. **propensity** [KPKS23]. **Properties** [DBE20, GOY20, HZG⁺20, SL20, SB20, ARR22a, ABAQ⁺23, AS20, BWS20, BA22, BMA⁺24, BSR22, BTSB22, CCZ23, CdSB⁺21, CM20a, CSG⁺21, CA22, DART21, DYGM21, HMK23, HD21, IW23, JS21, JMV21, KPPT21, KBHG23, LM24, LRF⁺21, LWF⁺22, LRKD23, LXP⁺22, LDT⁺22, dCB23, MMAZ⁺23, MCD22, NPGP23, OAN⁺23, PCB⁺24, PSM⁺20, PDP⁺24, PCI23, PSA⁺23, RMS⁺23, RMBSPJSG24, SBFSJMLU23, SGT⁺20, STB⁺20, VV20b, WSV20, WMJ⁺22, WYC⁺24, XDZ23, ZWL⁺24a]. **Property** [GZFSM21, DGS24]. **Property-oriented** [GZFSM21]. **propranolol** [IAS⁺24]. **propylene** [AMM22]. **protease** [BVC⁺23, dSCCN21, PWX⁺20, PPP21, UAC⁺23, YC23]. **proteases** [dMBdAVdS24, CBK⁺24]. **Protein** [BWM20, BSL20, CLS⁺20, HC21, LYKS23, MXM20, SZLD20, TWT⁺22, XZ20, ABTM22, AVM21, BK22, BPL⁺22, BBSFA22, BLB20, BAO⁺20, BF22, BVC⁺23, CDCT21, CH23, COK22, HTFY21, KCGK20, KR23, KGTL21, KSRKS21, KDP⁺22, KTM⁺23, LLS22a, LSP23, LL21b, LL22, MGB⁺22, MK22a, OC23, PDC23, PJJL23, QLW⁺22b, RDK⁺22, San21, SKL23, SY21, SEZ20, SLMA21, SNW22, WCY⁺24, WGKG20, YIO20, ENR⁺24]. **protein-glycosaminoglycan** [MGB⁺22]. **Protein-Ligand** [MXM20, LYKS23, TWT⁺22, KDP⁺22]. **Protein-Protein** [BSL20, COK22]. **protein-state** [BPL⁺22]. **Protein3D** [ENR⁺24]. **Proteins** [HHL⁺20, LJ20, BPDG21, CGSP24a, CCHS23, DB23, DO20, HB21, KCF⁺20, KOD21, LYKS23, LGC21, NYM22, POvG21, PPRS22, SSDL⁺23, TTH⁺21a, VWJ23]. **ProteinUnet** [KSRKS21]. **protic** [OM22]. **protocol** [ABNG22, Ben22, LCP21, LSC24, MPP23, MPV22, VWP⁺22]. **protocols** [PDP⁺24]. **Proton** [MFC20, AIV20, BBC20, BBBP⁺23, ĆNF23, DC22b, Nan24, RCC⁺20, SW21]. **proton-coupled** [ĆNF23]. **Protonated** [BAC20, MT21, ZHHS21]. **protonation** [CR24]. **protons** [LL21b]. **protoporphyrin** [KPR23]. **prototyping** [KRSD⁺23]. **provide** [UB20]. **proximity** [WCD⁺23]. **proximity-enforced** [WCD⁺23]. **Prp** [RDK⁺22]. **Pseudodiagonalization** [SM20]. **Pseudodiagonalization-based** [SM20]. **pseudoknots** [YFH⁺21]. **Pseudomonas** [VDK⁺20]. **Pseudopotentials** [KGTL21]. **Pseudospectral** [CHVF21]. **Psi4** [EK20a]. **PSIXAS** [EK20a]. **Pt** [DZL⁺20, PTP23, PPSP20, SS24, SVDS21, SSM21]. **pucker** [KB22]. **pull** [ARR22a, GPM21b, KdILC22]. **pulse** [LAM⁺23]. **pulses** [MLX⁺24]. **pump** [CGSP24a]. **pure** [BUNO22b, WTST24a, WMJ⁺22]. **purpose**

[BA24, BMT⁺²¹, Mar21]. **purposes** [DF22, PFPD21]. **push** [ARR22a, GPM21b, KdILC22]. **push-pull** [ARR22a, GPM21b, KdILC22]. **putative** [CDCT21]. **puzzling** [SVR⁺²⁴, XCJ20]. **Py3BR** [KWMPR24b]. **PyCDFT** [MWK⁺²⁰]. **PyFREC** [Kos22]. **PYK2** [SNW22]. **PyRad** [AME⁺²¹]. **pyranose** [KB22]. **pyrazinamide** [KMR⁺²⁴]. **pyrazine** [MH20]. **pyrazole** [BHR⁺²¹]. **pyrene** [JGdC⁺²³]. **PyRETIS** [RLR⁺²⁰, VZG⁺²⁴]. **pyridine** [PT21, PLT24, YFS20]. **pyrido** [MIP⁺²²]. **pyrimidin** [MIP⁺²²]. **pyrimidin-3-yl** [MIP⁺²²]. **pyrite** [KTBS23]. **pyrolysis** [KK22a]. **pyrrolylenones** [ARR22b]. **PySCF** [HAC^{+23b}]. **Python** [AKGD24, CM20a, DMD⁺²¹, KRSD⁺²³, LHH⁺²¹, MWK⁺²⁰, PSGL21, VAP⁺²¹, WRBT21]. **Python-based** [LHH⁺²¹]. **PyUNIxMD** [LHH⁺²¹]. **PyVisA** [AKR21].

Q [SK20, ZDBZ20, XZC⁺²⁴]. **Q-learning** [XZC⁺²⁴]. **Qball** [AME⁺²¹]. **QC** [KGD⁺²¹]. **QIDH** [RMBSPJSG24]. **QM** [Mar21, ABNG22, BBC20, GH22a, LRqG⁺²², LSCK23, Mar21, PWW20, PCI23, SSS^{+20a}]. **QM/MM** [ABNG22, BBC20, GH22a, LRqG⁺²², LSCK23, Mar21, PCI23, SSS^{+20a}]. **QM/QM** [PWW20]. **QM7b** [VT24]. **QM9** [VT24]. **QMCube** [Mar21]. **QSAR** [BHR⁺²¹, DF22, SS20]. **QSAR/MD** [HKFT21]. **QSARINS** [CSG⁺²¹]. **QSARINS-Chem** [CSG⁺²¹]. **QTAIM** [AMF⁺²⁰]. **quadrature** [IN23a]. **Quadruple** [Tze21, PTP23]. **Qualitatively** [Sts20]. **Quality** [RD23, AVM21, FB20, LB21, LB22, MK22a, SLB23]. **Quantification** [AWK⁺²³]. **quantify** [LKK⁺²³, Sch22b]. **quantifying** [IBL20]. **Quantitative** [AV20, BGS⁺²⁰]. **quantity** [RD23]. **quantized** [VCRP23]. **Quantum** [AWID⁺²⁰, IRB⁺²³, MMF⁺²⁴, Ooy20, PAS⁺²⁰, PHS⁺²⁰, Pil20, PSA⁺²³, SR23, AKGD24, AA20, BS23, BRNB21, BHR⁺²¹, BBK⁺²¹, CLTmd⁺²³, CSGVF⁺²⁰, CP23, FDK22, GPEK⁺²⁰, GP21, HKS20, HUUO23, HBT⁺²⁰, JCMHT22, JGGPN21, KRSD⁺²³, KFLP21, KB22, LGM20, LGM22, LYX⁺²², LCLB24, MLC⁺²³, OKI⁺²¹, OE20, Pwx⁺²⁰, PGP⁺²¹, RDB23, SPSH20, SSMP23, SIW21, SYS⁺²¹, SC23, SNN⁺²¹, Shi22, SKT24, dSSCC24, SCC⁺²², TPD21, TCS^{+21a}, VT24, VWJ23, XSP⁺²³]. **quantum-chemical** [BHR⁺²¹, SKT24, SCC⁺²², VWJ23]. **quantum-classical** [HUUO23]. **quantum-dot** [LCLB24]. **quasi** [Cer22, NSKN21]. **quasi-degenerate** [NSKN21]. **quasi-harmonic** [Cer22]. **quaternary** [ODL20]. **quaterthiophene** [CBF⁺²⁰]. **QuBiLS** [GJMPVR⁺²⁰]. **QuBiLS-MIDAS** [GJMPVR⁺²⁰]. **quest** [MMAZ⁺²³]. **quick** [Vyb23]. **quinoline** [RLHG⁺²³].

R [BR23, GGK20, LR20]. **R-1233zd** [BR23]. **R-1234yf** [BR23]. **R-32** [BR23]. **R-C** [LR20]. **R292K** [SSPK24]. **R61** [CD20]. **Rabenstein** [MDO⁺²⁰]. **radial** [CBF⁺²⁰]. **radical** [AFR^{+24a}, BA24, GNK⁺²³, MP23, OAN⁺²³, PFSC20, SKGG23]. **radical-mediated** [SKGG23]. **radicals** [KZ24, WKG⁺²³, ZYZ24]. **radii** [SHH^{+23a}]. **radiolysis** [AME⁺²¹]. **radon** [GH23]. **Raman**

[CV22, GPEK⁺20, MH20, OAN⁺23, PGP⁺21]. **Random**
 [HFPS20, VF20, YW20]. **Range** [BBK20, AS21, CHVF21, GH22a,
 GAP21, HTTT23, HTFY21, HCS⁺20, RMBSPJSG24]. **range-separated**
 [RMBSPJSG24]. **rank** [TXJT23]. **ranking** [PNT⁺22]. **Raphson** [MT20b].
Raphson/singular [MT20b]. **rapid** [LLZ⁺23, MT20b]. **rare**
 [RLR⁺20, RD23, VZG⁺24, ZWL⁺24a]. **Ras** [MM20]. **Rashba** [dARW⁺23].
rate [dCVARN20]. **rates** [CGMRVBAI22, GK24, KWMPR24b]. **Rational**
 [DSK21, SHP⁺23, ZZG⁺21, BXY⁺24, ZBH⁺23]. **ray** [EK20a, FB20]. **Rb**
 [SL20, AQMM⁺23, AQIS⁺24, RNP20]. **RBD** [KLZ⁺23]. **RC** \equiv [WLZM20].
RDFE [MPP23]. **R** \equiv [WLZM20]. **Reaction**
 [QB20, SLR⁺20, AMM22, BBY⁺21, BBC20, BCN22, CG20, CS20, CD20,
 CRT⁺21, DGS24, DWSX20, DPY⁺22, DLH⁺23, GSD⁺22, HL20,
 HREvdK⁺20, LLS⁺22b, LRqG⁺22, LBH⁺22, MNZGO⁺20, MIP⁺22,
 MNBG⁺21, MA23b, NAAP21, PRF20, PDP⁺24, PM21, SYS⁺21, SSS⁺20a,
 SKGG23, SSM21, SCZ⁺21, TYZ20, XZC⁺24, YGG⁺23, ZLLL22, ZS22].
Reactions [ĆNF23, OOY20, SK20, ABZ20b, BAM⁺24, BBBP⁺23, GCP22,
 LSC24, LHG⁺23, MH22, MDO⁺20, MN20, PRF20, RCC⁺20, SKY24,
 SYS⁺21, SC23, SMB⁺23, SSYB⁺20, WKCP21, dCVARN20]. **Reactive**
 [TSH⁺23, BJ22, FVSS20, PSW⁺24, ZG21]. **Reactivities** [MML⁺23].
Reactivity [SHM⁺20, VAL20, BA24, CMD⁺22, GM22, KFLP21, KTBS23,
 LGJF22, LMPT21, MAI22, ZS22]. **reading** [VAP⁺21]. **reagents** [SCZ⁺21].
Real [MSS20, CCPR24, GCP22, HAC⁺23b, KdILC22]. **Real-time**
 [MSS20, CCPR24, HAC⁺23b]. **Realistic** [IN23b, ZWY⁺22]. **reality**
 [MSL⁺20]. **Realization** [SH23]. **Rearrangement** [PGP⁺23]. **reason**
 [RTB23]. **Reasoning** [QB20]. **ReaxFF** [WW24]. **Receptor**
 [BWM20, BRNB21, BHR⁺21, CSP20, TPZ⁺20, TZS⁺22, VWP⁺22, WGKG20].
receptor- [CSP20]. **receptor-flexible** [VWP⁺22]. **Receptor-Membrane**
 [BWM20]. **Receptors** [Min20]. **recognition**
 [BPL⁺22, BRNB21, DPSG20, KGD⁺21, SCCZ21, WCT⁺23]. **Recognizing**
 [HGF20]. **recombination** [KWMPR24b]. **reconstruction**
 [ABTM22, PPV⁺21]. **reconstructions** [OAC23]. **Record** [HZG⁺20].
Recovering [RGGD21]. **recovery** [DK23]. **rectangular** [AYO20].
recurrence [Gao20, IN23a]. **recurrence-relation** [Gao20]. **recurrent**
 [TIK21]. **Redox** [RvWH23, AFR⁺24a, Cha24, MLB⁺23, RLHG⁺23, SM22b].
Redox-active [RvWH23]. **reduced** [Ore24]. **reductase** [CFOMCB⁺22].
Reduction [ABZ20b, AR20, MC24, NAAP21, PPSP20]. **reference**
 [BTSB22, KWYN23, VM23, WKL22]. **references** [LWC⁺24]. **Refined**
 [KSRB⁺21]. **refinement** [NSRK21, RCC21]. **regime** [FCPG20]. **regio**
 [BXY⁺24, SMB⁺23]. **regio-** [BXY⁺24, SMB⁺23]. **region** [FKT21]. **regions**
 [HTTT23, SSPK24]. **Regioselective** [JFZ⁺20]. **Regioselectivity** [JFZ⁺20].
regression [BP22, MP24, OKK22, SS23]. **regularized** [SS23]. **regulating**
 [PPRS22, WSV20]. **regulator** [CDCT21]. **Reinforcement**
 [LHB⁺24, JGK⁺22]. **related** [BPL⁺22, CdSB⁺21, MLB⁺23]. **relation**
 [Gao20]. **relationship** [HS22]. **relationships** [MML⁺23]. **relative**

[MPP23, PWX⁺²⁰, ZQ24]. **Relativistic** [GH22b, GH23, IWN24, KWYN23, MCD22, RNP20, SDK20]. **relaxation** [GNK⁺²³]. **release** [GGK20, Gie21, PRH20]. **relevant** [DF22, GKA^{+23b}]. **Reliability** [ZWR22, Sch22b]. **Reliable** [PFSC20, AD23, CK22, LWC⁺²⁴]. **reliably** [APP24]. **REMD** [MGB⁺²²]. **removal** [FNY21]. **renewable** [LM24]. **renormalization** [BBK⁺²¹, TT20, XSP⁺²³]. **repair** [CGMRVBAl22]. **Replacement** [ZXD20a, ZXD20b]. **replica** [FYIO23, JKS23, KN21, MGB⁺²², MZMK⁺²¹, RR22, SEZ20]. **replicas** [SDH23]. **repositioning** [SLMA21]. **Representation** [WZZ⁺²⁰, BLB20, DF22, OKK22, WCY⁺²⁴]. **Representations** [Bal20a, SBG20, CN21]. **repulsion** [KDLP21]. **repulsion-corrected** [KDLP21]. **repulsive** [MGB⁺²², MZMK⁺²¹, SEZ20]. **repurposed** [PPRS22]. **Repurposing** [EIT⁺²¹]. **residue** [BPL⁺²²]. **residues** [MAP⁺²⁰]. **resistance** [BF22, SSPK24]. **resolution** [IAF⁺²⁴, LSP23]. **resolved** [AS21, ABNG22, CS23, KRW⁺²⁴]. **Resolving** [WdGG24, XCJ20]. **Resonance** [OAN⁺²³, WG21, AV20, ARR22b, ERVN24, LL21b, NHFS21, Wan21a, Wan21b]. **resonance-assisted** [AV20, ARR22b]. **resonances** [BBY⁺²¹]. **resource** [LGD⁺²⁰]. **respect** [CC22]. **Response** [MLX⁺²⁴, Wan21a, CC22, KZ24, Tou21]. **responsive** [KCF⁺²⁰]. **Restoring** [WKD⁺²¹]. **restrained** [QLC⁺²⁰]. **restrained-ensemble** [QLC⁺²⁰]. **Restrains** [MXM20]. **Results** [BdLC21, Sts20]. **retinal** [GK24]. **revealed** [LHG⁺²³]. **revealing** [ARR22b, HTTT23]. **reveals** [BPDG21, HREvdK⁺²⁰, JRS20, MAM21, ONA⁺²⁰, SSPK24]. **Review** [ZFRM20]. **revisited** [NSH23, PC23, SWF⁺²⁰, TTT⁺²¹]. **Revisiting** [MMAZ⁺²³, SCZ⁺²¹]. **RhB** [Tze21]. **rhencyclopropene** [DZ23]. **rheology** [NP23]. **Rhodopsins** [HREvdK⁺²⁰]. **riboswitches** [AAe20]. **ribozyme** [JRS20]. **rich** [JMV21, SCCZ21]. **Riemann** [MA23a]. **right** [SCZ⁺²¹]. **Rigid** [Min20, WCD⁺²³]. **Ring** [LJ20, AG21, Jab22b, KB22]. **rings** [DZ23, HS22, HS23]. **RISM** [CKH23, MY24, YIO20]. **RISM/3D** [MY24]. **RISM/3D-RISM** [MY24]. **RISMicCal** [MY24]. **RL** [JGK⁺²²]. **Rn** [APR21]. **RNA** [AAe20, BVGB23, KR23, SCCZ21, TM20, WCT⁺²³, YFH⁺²¹]. **robust** [NMF121]. **Role** [MKSS20, MAP⁺²⁰, NAAP21, BVC⁺²³, FM21, GCP22, KE23b, LKT21, MCD22, SGGG22, SNK24b, ZG21, ZOD⁺²²]. **roles** [VV20b]. **rotamers** [PFP⁺²¹]. **rotating** [YrYqLhC23]. **rotation** [Kop22b, PGDD24]. **rotational** [PSMPB21]. **rotations** [PDL24]. **rotors** [YrYqLhC23]. **route** [SSM21]. **Roux** [IBL20]. **rovibrational** [ERVN24, IAF⁺²⁴, SR23]. **RS** [MGB⁺²², SHHH22, VAL20]. **RS-REMD** [MGB⁺²²]. **RSX** [RMBSPJSG24]. **RSX-QIDH** [RMBSPJSG24]. **Ru** [HSG21, CPP⁺²²]. **rubber** [MML⁺²³]. **RuBisCO** [DGSB⁺²⁰, JMK⁺²⁰]. **RuC** [Tze21]. **rule** [TLD⁺²², TTT⁺²¹]. **rung** [RMJ21]. **rung-3.5** [RMJ21]. **ruthenium** [KK23, YYS20]. **rutile** [VTdlM20].

S [DBE20, GCP22, Gie21, SLR⁺²⁰, PWW20]. **SA** [Sts20]. **SA-2-CASSCF**

[Sts20]. **saddle** [MH22]. **safe** [JRS20]. **salts** [JMV21]. **same** [Sán20]. **same-spin** [Sán20]. **Sampling** [FMFG20, RD23, AKR21, BPT⁺23, FYIO23, GVJ⁺22, KN21, KSRB⁺21, LGC21, Ngo21, PPV⁺21, SBD⁺21, SSS⁺20a, STR20, WLSC23a, ZGZC20, ZKJ⁺23]. **sandwich** [AS23, KBHG23]. **SARS** [dMBdAVdS24, EIT⁺21, KLZ⁺23, ONA⁺20, PDC23, PPP21, PPRS22, SLMA21, UAC⁺23, YC23]. **SARS-CoV-** [SLMA21]. **SARS-COV-2** [ONA⁺20, dMBdAVdS24, EIT⁺21, KLZ⁺23, PDC23, PPP21, PPRS22, YC23]. **save** [POvG21]. **scalar** [RNP20]. **scale** [ARR22a, BTC24, BGS⁺20, CJHW21, HREvdK⁺20, JKK⁺21, LSC⁺23, RDS⁺20, SY21, UAC⁺23, YMM⁺24]. **scaled** [Sán20]. **scaling** [ASW20, CC22, MKK⁺22, MGB⁺22, MZMK⁺21, RR22, SEZ20, ZWY⁺22]. **scandium** [GSSG24]. **scattering** [CV22, DHD21, MH20]. **scavenger** [Mon24]. **SCF** [HNCL24]. **SCH** [SVTK⁺22]. **scheduling** [MLC⁺23]. **Scheme** [BSL20, GRN20, BA24, FCPG20, Gao20, LLZ⁺23, MT20b, RH21, STR20, VWJ23, ZZ23a]. **schemes** [DO20, HD21, MPP23, SFS24, ZQ24]. **schiff** [ZRSST20]. **Schrödinger** [Nan24]. **Schwarz** [IW23]. **Science** [PAF⁺20, PSGL21]. **Scope** [TZS⁺22]. **Scoring** [LAM⁺23, AMF⁺20, KDP⁺22]. **Scorpionates** [FNPD22]. **scramblase** [KCF⁺20]. **screened** [YW20]. **Screening** [ZYZ24, AFR⁺24a, AR20, CJHW21, KDP⁺22, LCP21, MLG⁺21b, MPR22, NBE⁺23, Ore24, UAC⁺23, WRVP22]. **Se** [JS21, KPTT21, AQMM⁺23]. **Search** [BW22b, BAO⁺20, RD24, TIK21]. **Searching** [DTA21, ZDBZ20]. **second** [CC22, CSGVF⁺20, FKT21, GX20, Sán20, YW20]. **second-order** [CSGVF⁺20, FKT21, GX20, Sán20, YW20]. **Secondary** [AD20, AAe20, HC21, JRS20, KSRKS21]. **sections** [ALA20, CV22, dBCdL20]. **seen** [CCZ23]. **selected** [CN21, KZOV23]. **selected-CI** [CN21]. **selection** [BPL⁺22, LCP24, SKL23]. **selective** [HRTSS⁺20, KI24, YLZ⁺22, ZOD⁺22]. **selectivity** [BAM⁺24, FDD⁺23, KPKS23, MIK⁺23, NMMC21, SMB⁺23, SKGG23]. **selenium** [ZGZ⁺20]. **selenium-containing** [ZGZ⁺20]. **selenolate** [KPTT21]. **Self** [IW24, ASW20, BUNO22b, CV22, CQSG20, CTPJH22, MAP⁺20, PRH20, SKKK20]. **self-assembly** [MAP⁺20, PRH20]. **Self-consistent** [IW24, CV22, CQSG20, CTPJH22, SKKK20]. **self-diffusion** [BUNO22b]. **self-interaction** [ASW20]. **semi** [KB22, PWX⁺20, RLHG⁺23, TV22]. **semi-empirical** [KB22, PWX⁺20, RLHG⁺23]. **semi-local** [TV22]. **semiclassical** [FCB23]. **semiconducting** [CBF⁺20, KPHV23, LHC⁺21]. **semiconductor** [LMPT21, WMJ⁺22, ZGZ⁺20]. **Semiempirical** [GUCCR20, Gie21]. **Sensing** [HRTSS⁺20]. **Sensitivity** [BTSB22, LGM20, MM24]. **sensitizers** [LCP21]. **sensor** [ZRSST20]. **sensors** [MK22b]. **Separated** [BBK20, RMBSPJSG24]. **Separation** [NS22, WG20, YYZ⁺21, ZHG⁺24]. **SEQCROW** [SIW21]. **sequence** [CR24, KZOV23, KSRKS21, SBFSJMLU23]. **sequence-based** [KSRKS21]. **sequential** [GGK20]. **series** [BHR⁺21, PWX⁺20, WZW⁺24, ZWL⁺24a]. **server**

[LGD⁺20, MPuS⁺20, FPMD23]. **servicing** [TSH⁺23]. **Set** [XZ20, YXGZ20, BK22, Fed24, HGR⁺24, KS21, MM24, MCP23, SCKH21, TAC⁺23]. **sets** [GZFSM21, GH22b, GH23, KM24, LB21, LB22, NSH23, RNP20, SLB23, SM22a]. **setup** [CLTMd⁺23]. **seven** [KZJ22, ZYZ24]. **seven-electron** [ZYZ24]. **seven-membered** [KZJ22]. **sextet** [TLD⁺22]. **sH** [MJS⁺23]. **Sham** [BTSB22, EK20a, HCS⁺20, MB21]. **shape** [KTM⁺23]. **SHARK** [Nee23]. **Shavitt** [SBG20]. **sheets** [SS23, XIV⁺24]. **shell** [AME⁺21, GSSG24, IW24, Klo22, MB21, Sán20, SM23, PSMPB21]. **shielding** [CMG⁺24]. **shift** [FBP⁺22, TTDT20, UB20]. **shifts** [Ben22, KWX23, MPV22, ZHHS21]. **shock** [BAO⁺20, FVSS20]. **short** [HTFY21, SKKG22]. **short-range** [HTFY21]. **Si** [GPM21b, WMJ⁺22, KPR23, WTST24a, VCRP23]. **side** [BSR22, ODL20, SSS⁺20b]. **side-chain** [SSS⁺20b]. **signal** [XIV⁺24]. **signaling** [CDCT21]. **sil** [KDMM24]. **sil/germa** [KDMM24]. **silaboryne** [DDSM23]. **silane** [MML⁺23]. **silica** [MML⁺23]. **silica/rubber** [MML⁺23]. **silico** [dMBdAVdS24, LHB⁺24, MAI22, SEBE21, SC23, PFPD21]. **Silicon** [HZG⁺20, GPEK⁺20, PGP⁺21, WZW⁺24, ZXD20b, ZXD20a]. **silicon-based** [WZW⁺24]. **siloxo** [LLS⁺22b]. **silver** [FNPD22, Mon24, XDZ23]. **similar** [HGF20]. **similarity** [WRVP22]. **Simple** [RH21, BW22a, BK22, Shi22, VWJ23]. **Simplex** [WSL⁺20]. **simplify** [CTPJH22]. **simulate** [ABNG22, LRqG⁺22, TTH⁺21a, TMO⁺21]. **simulated** [CS23]. **Simulating** [LA20, AME⁺21]. **Simulation** [HZG⁺20, NNT⁺20, PAF⁺20, RR22, SL20, SNW22, ZHG⁺24, BBC20, BP22, CDCT21, CSP20, CBB⁺21, FNY21, GG22, HREvdK⁺20, HBM⁺20, KCGK20, KGS⁺22, KLP⁺22, NLC23, NP23, ONA⁺20, PPP21, RKC21, SYS⁺21, SNN⁺21, SY21, SWLC22, SCCZ21, UKBD23, VWFR21, YC23, YWGY22, ZK21]. **simulation-based** [CDCT21]. **Simulations** [SZLD20, Zac20, BUNO22b, BTL24, CCZ23, DO20, EK20a, FCB23, FLT23, GGK20, HUUO23, IAS⁺24, JKS23, LL21a, LKM20, LSC⁺23, LGC21, MP24, MPOC21, MSA22a, Ngo21, NN20, NP23, PDC23, PBM21, PDL⁺21, POvG21, PL22, PCI23, QLC⁺20, RDK⁺22, RGGD21, SC23, SSDL⁺23, SKKK20, TTK23, TPB22, Tik23, WCT⁺23, WW24, WGKG20, WFBB22, WKD⁺21, Yos24, YMM⁺24, ZKJ⁺23]. **Simultaneous** [GKO⁺22, BMT23, WFLZ23]. **single** [AK20, BW22a, CBF⁺20, DLH⁺23, EVKL21, FMK24, GSD⁺22, KSRKS21, VM23]. **single-** [VM23]. **single-electron** [EVKL21]. **single-ended** [GSD⁺22]. **single-molecule** [AK20]. **single-walled** [BW22a, CBF⁺20]. **single/dual** [DLH⁺23]. **single/dual-atom** [DLH⁺23]. **Singlet** [HFPS20, FCB23, LCP21, MdSJ⁺23, SCKH21]. **singular** [MT20b]. **Site** [VDK⁺20, BBC20, CDCT21, CCHS23, DPSG20, KWYN23, KGD⁺21, PLP⁺20, TZS⁺22, WKL22]. **site-specific** [CCHS23]. **sites** [ENR⁺24, HGF20, LKM20, MAKZ23, TXJT23, VHS⁺24, YIO20]. **sites-based** [VHS⁺24]. **Si** \equiv [DDSM23]. **situ** [MC24, WKG⁺23]. **situation** [FNPD22]. **situations** [THLC⁺23]. **six** [PTP23]. **six-electron** [PTP23]. **sixth** [LB21]. **size**

[GH22b, GH23, HKS20, JS21, KPR23, LBH⁺22, SSSA23, XAD20]. **size-modified** [XAD20]. **Sized** [MFC20, BSS⁺22, ZDBZ20]. **slab** [VTdlM20]. **Slater** [DWZ22, FV20, HNCL24, MFS22]. **Slater-type** [MFS22]. **sliced** [GVJ⁺22, KN21, PPV⁺21]. **slip** [WKD⁺21]. **slip-springs** [WKD⁺21]. **slow** [VZG⁺24]. **Sm** [ALA⁺22]. **Small** [KDMM24, LPP20, Mil21, SLML24, GH22b, GH23, JS21, KYM20, LPF⁺23, MLP22, MC24, Mon24, NST⁺20, SKL23, TIK21, WLWR22, YIO20, ZK23, ZDBZ20]. **small-molecule** [ZK23]. **small-sized** [ZDBZ20]. **Smoothed** [GJMPB⁺20]. **Sn** [LXP⁺22, WTST24a]. **sodium** [NSH23, SM22b]. **Soft** [SJA24]. **Soft-sphere** [SJA24]. **softness** [MAI22]. **Software** [Kos22, Zac20, AG21, AME⁺21, CKH23, CJHW21, CSG⁺21, DMD⁺21, GJMPVR⁺20, HAC⁺23b, KWMPR24b, LHH⁺23, MLG⁺21b, MY24, RBM⁺23, SNN⁺21]. **solar** [SZP⁺20, TANC23]. **Solid** [TPD21, EG20, HM21, LB21, LB22, LZW⁺23, SLB23, UKBD23]. **Solid-state** [TPD21, LB21, LB22, SLB23, UKBD23]. **solids** [CdSB⁺21]. **solubility** [BR23, FLT23, WCY⁺24]. **Solute** [GRN20, JKS23, KN21, ZKJ⁺23]. **solution** [KGS⁺22, KK23, KTM⁺23, MPOC21, PGH24, RPD⁺20a, SH23]. **solutions** [ĆNF23, KSS21b, KSRB⁺21, SSS⁺20a]. **solvated** [LRKD23, MSA22b]. **Solvation** [GRN20, LPF⁺23, MFC20, BSB⁺24, CKH23, CCHS23, GRBN21, GSH23, LML⁺23, NML21, RPD⁺20a, RB24, SJA24, SHH⁺23a, VL22, VV21, Vyb23, WKL22]. **solve** [BSB⁺24, MA23b]. **Solvent** [BBK20, FMFG20, GCL⁺20, KWYN23, SLR⁺20, Sts20, BAM⁺24, CMG⁺24, CDCT21, DK23, KLC⁺24, KK23, KPHV23, LML⁺23, MLM⁺24, MGB⁺22, PT21, SPSH20, SHHH22, VCL20, WLSC23a, XAD20]. **solvent-accessible** [VCL20]. **solvents** [Ore24, OM22, RPD⁺20a, SJA24, VV21]. **solver** [NSRK21, VHS⁺24, WK21]. **solvers** [UYJ⁺24]. **solving** [MB21]. **Some** [QB20, MAI22]. **sorbitol** [KSS21b]. **source** [AAID22, FR21, HAC⁺23b, MNBG⁺21, PSGL21, RBM⁺23]. **sp** [AKN⁺20, PPP21]. **space** [BPT⁺23, BAO⁺20, GCP22, HL20, KZOV23, MPR22, PJJL23, RSHG23, SBD⁺21, TZS⁺22]. **spaces** [UR23]. **SPANNA** [YMM⁺24]. **Sparse** [BPL⁺22]. **Spatial** [YMM⁺24]. **speciation** [LGD⁺20]. **species** [KDMM24, XAD20]. **specific** [CCHS23, WRBT21, ZKJ⁺23]. **Spectra** [CWZD20, CS23, EK20a, GPEK⁺20, IAF⁺24, KGS⁺22, KBK⁺24, LWLC21, OAN⁺23, PGP⁺21, SNK24b, SNN⁺21, TMO⁺21]. **spectral** [LDT⁺22]. **spectroscopic** [LZW⁺23, PYA24]. **Spectroscopy** [BLP20, CMD⁺22, FB20, KF24, MPOC21, Sai23]. **spectrum** [AS21, SS24]. **speed** [GWN21, WFBB22]. **sphere** [SJA24]. **Spherical** [GJMPB⁺20]. **SPIDER3** [KSRKS21]. **SPIDER3-single** [KSRKS21]. **spike** [Jab22b, ONA⁺20, PDC23]. **spike-ring** [Jab22b]. **Spin** [IYI⁺20, SWF⁺20, SWM⁺20b, TPD21, GNK⁺23, HYA⁺20, KE23b, KKAK23, NBE⁺23, PDGD23, PHS⁺20, POPGS22, QLC⁺20, Sán20, UR23, VV20b, WTST24a, XCJ20]. **spin-adapted** [UR23]. **spin-coupled** [XCJ20]. **Spin-flip** [IYI⁺20, KKAK23]. **Spin-inversion** [SWF⁺20, SWM⁺20b]. **Spin-liquids** [TPD21]. **spin-mixed** [WTST24a]. **spin-orbit** [PHS⁺20, POPGS22]. **spin-pair** [QLC⁺20]. **spin-polarized** [NBE⁺23].

spin-pure [WTST24a]. **spiropyran** [DK23]. **splicing** [SCCZ21]. **splitting** [OSHT20, YYS20, dARW⁺23]. **splittings** [SRB21]. **Spontaneous** [PRIP24]. **SPOT** [CLS⁺20]. **SPOT-Fold** [CLS⁺20]. **springs** [WKD⁺21]. **SrC** [SGSB23]. **stabilities** [WKCP21]. **Stability** [GKA⁺23b, STB⁺20, VAL20, APR21, BK22, BGPR24, BPDG21, CCHS23, DDSM23, GM22, KZ24, LML⁺23, MVV22, MdSJ⁺23, MJS⁺23, MIP⁺21, NLC23, PDC23, PB20, PLT24, PP23, VTdlM20]. **Stabilization** [BD22, GPM21b, FM21, PFSC20]. **stabilized** [KW22, PLZT23, WCD⁺23]. **stabilizing** [DSB23]. **stacking** [XLW⁺22]. **Standalone** [KYM20, CSG⁺21]. **standard** [KM24, TZS⁺22]. **stannites** [MZ21]. **stannylenes** [BKM21]. **stars** [GSJ⁺23]. **State** [BWM20, BSF20, AST24, AIV20, BPL⁺22, CH23, FYIO23, HNCL24, HD21, HPM⁺21, KL20, KWB24, KBHG23, Kop22b, LB21, LB22, LHH⁺21, OSHT20, OAN⁺23, RSHG23, RLHG⁺23, SLB23, Sts20, TPD21, Tou21, UKBD23, VHS⁺24, WD20, WMZJ20, XZC⁺24, ZRSST20, dCVARN20]. **State-of-the-art** [BSF20]. **states** [BGPR24, BMT23, BW22b, CG20, CPG21, CCPR24, EVKL21, FCB23, FB21, FMK24, Gie21, HYA⁺20, IK21, JCMHT22, Kop22a, LJW⁺23, MdSJ⁺23, NBE⁺23, OMC⁺20, RDS⁺20, SDH23, SBB⁺22, SHH⁺24, VM23, WFLZ23]. **static** [BBBP⁺23, EVKL21]. **Statistical** [AAe20, DC22b, UKBD23]. **steady** [VHS⁺24]. **steady-state** [VHS⁺24]. **steels** [ZFRM20]. **steered** [MK22a]. **step** [AFR⁺24a, FR21, POvG21, WKG⁺23]. **step-length** [FR21]. **stepping** [MKK⁺22]. **stepping-based** [MKK⁺22]. **steps** [DGSB⁺20]. **stepwise** [BBBP⁺23, KZJ22]. **stereo** [SMB⁺23]. **stereographic** [VCL20]. **Stereoselectivity** [WLZM20, DRBT24]. **Steric** [VDK⁺20, GCP22]. **stiffness** [MA23b]. **stochastic** [SSFS22b]. **stone** [CTBB20]. **stone-wales** [CTBB20]. **storage** [SKKG22, SSYB⁺20, WG20]. **story** [SVR⁺24]. **Strain** [SLR⁺20, MGCM21]. **strains** [LSC⁺23]. **Strategies** [PDGD22, PFPD21, SBB⁺22]. **strategy** [dMBdAVdS24, HB21]. **streamline** [PBM21]. **strength** [CVGVN⁺20, FDD⁺23, MVP⁺20, NTK21]. **Streptomyces** [CD20]. **stretching** [GAP21]. **strong** [FCPG20]. **strongly** [BA24]. **strontium** [KGG21]. **Structural** [ABAQ⁺23, CM20b, MdSJ⁺23, PSM⁺20, SL20, WMJ⁺22, AVM21, FPMD23, LM24, ONA⁺20, PYA24, QLW⁺22b, SH23, XZW⁺21, ZOD⁺22]. **Structure** [CLS⁺20, GLC⁺22, GG22, MJS⁺23, MIP⁺21, NLC23, WCD⁺23, XZ20, AAe20, ABTM22, AYO20, BLB20, CMO⁺24, CGSP24a, Che23, DGSB⁺20, JX24, GH22a, GSD⁺22, GAG20, HC21, HSG21, HGF20, KWYN23, KDKS21, KPDB22, KDP⁺22, LSP23, LL21b, MNH21, MZ21, MPV22, MK22a, NUK21, NHFS21, NDK24, PJJL23, PDGD22, PP23, RKC21, RDK⁺22, RvWH23, SS24, SM22b, UR23, VTdlM20, VM23, WS21, XZW⁺21, ZWY⁺22]. **structure-** [GH22a]. **structure-based** [GLC⁺22, KDP⁺22, LSP23, RKC21]. **structure-guided** [CGSP24a]. **Structures** [CWZD20, HZG⁺20, LWF⁺22, PLT24, ZBH⁺23, AAID22, AZKM22, Ari24, CR24, DC22a, DTA21, DYGM21, KS21, KZP22, KGTL21, KSRKS21, LSP23,

LXP⁺22, LHB⁺24, LL22, MH22, NSKN21, POPGS22, SGSB23, SFS24, SAZ⁺23, TT20, WHJM23, YIO20, ZDBZ20, ZWR22]. **studied** [LL21a, SY21, WS21]. **Studies** [CWZD20, ARA22, BR23, CFOMCB⁺22, CX21b, CMD⁺22, DA22, FPMD23, GM22, HKSW20, LM24, LGJF22, LCLB24, MSE⁺21, MSA22a, NLC23, RKC21, RR22, ZFRM20]. **Study** [AQRA⁺23, JFZ⁺20, KBK⁺24, ARR22b, APS20, AMM22, ALA⁺22, BW22a, BA22, BXY⁺24, BBC20, BA24, BEKM24, BD22, CS20, CL23, CTBB20, CCPR24, CRT⁺21, DSS⁺24, DZL⁺20, DK23, DLH⁺23, DSK21, FDK22, FAK24, HS22, HM21, HTFY21, HSG21, HCY⁺22, IAS⁺24, JC20, JAP⁺24, JMV21, KZJ22, KR23, KM22, KLC⁺24, KBHG23, KSRB⁺21, KEK23, KPKS23, LLJ⁺24, LSC24, LEP⁺21, LC22, LJW⁺23, MNH21, MNZGO⁺20, MLP22, MAP⁺20, NAAP21, NAN⁺23, NPGP23, OE20, OSM20, PRH20, Pan23, PDGD23, PLT24, PM21, RPD⁺20a, RDS⁺20, SGRN24, SEBE21, dASRHB21, SVDS21, SSS⁺20a, SI22, SC22, SKT24, dSSCC24, TANC23, TMO⁺21, TLS23, TPZ⁺20, VTdlM20, WTST24a, WG20, WRBT21, WKG⁺23, YSMS24, YYS20, ZDBZ20, ZMH⁺21, ZG21, ZHG⁺24]. **studying** [RDB23]. **style** [Tik23]. **styrene** [ZZG⁺21]. **sub** [NAAP21]. **subject** [LAM⁺23]. **subnanoclusters** [FBM⁺23]. **suboxide** [LZW⁺23]. **substances** [MHA⁺23, MVV22]. **substituent** [BMA⁺24, CMO⁺24, JK21, LGM20, LGM22, MAM21, dCB23]. **substituents** [JGdC⁺23]. **Substituted** [NRH⁺20, ASL⁺20, BSR22, CCPR24, KBK⁺24, MNZGO⁺20, NMMC21, SW21, SMB⁺23]. **substitution** [ĆPP⁺22, HREvdK⁺20, JC20, TAB⁺24]. **Substitutional** [GPEK⁺20]. **substrate** [LHB⁺24]. **substrates** [KCF⁺20, PDP⁺24]. **sugar** [SGGG22]. **suitable** [SHH⁺23a]. **suite** [Mar21]. **sulfide** [MSE⁺21]. **sulfur** [SaATR24]. **sulfuric** [KEK23]. **summation** [Pan23, WKL22, YLZ⁺20]. **superacids** [Brz23]. **Superalkalis** [Mil21]. **Superatom** [VKSS24, YMSS23]. **supercomputer** [JKS23]. **superconductors** [TPD21]. **Superfamily** [MM20]. **superhalogens** [Mil21]. **superphane** [Jab22a]. **Superposition** [Wan21a, Wan21b, WG21]. **supersalts** [Mil21]. **superstructures** [TPD21]. **supported** [BWS20, DZL⁺20]. **supramolecular** [GBM20]. **Surface** [GCL⁺20, MH20, PAF⁺20, YXGZ20, ERVN24, FCPG20, IW23, KTBS23, LHG⁺23, MSE⁺21, OKI⁺21, PM21, SZP⁺20, SSM21, THH⁺24, TV22, VCL20, WK21, XLW⁺22, XZC⁺24]. **Surface-enhanced** [MH20]. **surfaces** [APP24, AWK⁺23, DA22, HPM⁺21, LMPT21, MN20, MSL⁺20, OKK22, PCB⁺24, RDB23, Sts20, VCL20, WTST24a]. **surrounding** [Sch22a]. **survey** [MLGY24]. **SuSMoST** [PAF⁺20]. **swarms** [LA20]. **switchable** [KFTB20b]. **symmetry** [BPDG21, NTK21, NVBG23, OE20, PSMPB21, SNK24b, SM22b]. **symmetry-adapted** [NTK21, OE20]. **symmetry-decomposed** [NVBG23]. **synergistic** [PRH20]. **Synergy** [HLV⁺24]. **Synthesis** [MSE⁺21, KZJ22, SEBE21]. **System** [HHL⁺20, NAN⁺23, DGM22, Nee23, PDL24]. **Systematic** [IWN24, KUNT20, STR20, DSK21, SKT24, TS21]. **Systems** [LR20, AAID22, JGdC⁺23, EVKL21, GNK⁺23, HAC⁺23b, IW24, JKK⁺21,

JKS23, LC22, dCB23, NLC23, PSW⁺²⁴, PKT21, SIW21, dSSCC24, THH⁺²⁴, UB20, WG20, YAO20].

T [CS20, CK22, CSWW20, Dor20, KG23, MLB⁺²³, MEKH22, PRF20, SI22, SGSB23, GG22, Sts20]. **T-peptide** [GG22]. **T1** [MCP23]. **Taba** [dSBFdAJ20]. **TABI** [WK21]. **table** [GWN21]. **TaH** [WLZM20]. **tailoring** [AV20, ARR22a, ARR22b]. **Taking** [GNL⁺²²]. **tangential** [CBF⁺²⁰]. **target** [KR23, SLMA21]. **targeted** [CGSP24a]. **targeting** [CBK⁺²⁴]. **targets** [BF22]. **task** [DRBT24]. **TATA** [SBFSJMLU23]. **TATA-DNA** [SBFSJMLU23]. **tautomeric** [CA22]. **tautomerism** [LKAT22]. **Tautomerization** [NHFS21]. **TBP** [WCT⁺²³]. **TcN** [Tze21]. **TD** [ABNG22, DK23, LDT⁺²², MPOC21, MK22b, WD20]. **TD-DFT** [ABNG22, DK23, LDT⁺²², MPOC21, MK22b]. **TDDFT** [HAC^{+23b}, NRH⁺²⁰, Sts20]. **TDP** [SCCZ21]. **TDP-43** [SCCZ21]. **Technique** [WSL⁺²⁰, NP23]. **techniques** [MZ21]. **technology** [AQIS⁺²⁴]. **Teller** [PGDD24, PDL24, Tou21]. **Temperature** [XZW⁺²¹, GVJ⁺²², PPV⁺²¹]. **temperature-accelerated** [GVJ⁺²²]. **Temperature-dependent** [XZW⁺²¹]. **tempering** [JKS23, KN21, LGC21]. **tendency** [MSA22a]. **tension** [MK22a]. **tensor** [GJMPVR⁺²⁰, OKK22]. **Terminal** [JFZ⁺²⁰, MKSS20, SK23, CCZ23, Ano24a]. **termini** [XIV⁺²⁴]. **terms** [GKO⁺²², MR21]. **terthiophene** [KBK⁺²⁴]. **test** [SHH^{+23b}, SHH^{+23a}]. **Testing** [KM24, KG23, NGD22]. **tetra** [BR23, dSCCN21]. **tetra-coordinate** [dSCCN21]. **tetrabutyrates** [BR23]. **tetrachloro** [SHH⁺²⁴]. **tetrachloro-** [SHH⁺²⁴]. **tetracoordinate** [DC22a]. **tetrafluoride** [Brz22]. **tetrafluoro** [BR23]. **tetrahedral** [BA22]. **tetrahydro** [MSE⁺²¹]. **tetrahydro-** [MSE⁺²¹]. **tetrahydrodibenzazosines** [SS20]. **tetrakis** [MVP⁺²⁰]. **tetranuclear** [KKAK23]. **tetraoctanoate** [BR23]. **tetrapeptide** [MAP⁺²⁰]. **tetrasulfonyl** [DART21]. **tetravalent** [SDK20]. **tetrel** [Brz22]. **Tf** [TYZ20]. **TGR5** [WGKG20]. **their** [DC22a, MK22b]. **theophylline** [TM20]. **theophylline-RNA** [TM20]. **theorem** [GX20]. **theoretic** [TAC⁺²³]. **Theoretical** [BMA⁺²⁴, DA22, GSSG24, JMK⁺²⁰, LGJF22, MML⁺²³, VTdM20, AQMM⁺²³, BD22, BBL⁺²², HRTSS⁺²⁰, HSG21, KDKS21, KK22a, KBK⁺²⁴, MNZGO⁺²⁰, MLGY24, NMFI21, OSM20, PRH20, RPA⁺²⁴, TSH⁺²³, YSMS24, ZS22, ZWL24b]. **theories** [KK23]. **Theory** [CC22, IYI⁺²⁰, SK20, YXGZ20, APS20, AS21, ASL⁺²⁰, ABAQ⁺²³, AA20, BWS20, BA22, Ben22, CFOMCB⁺²², CHVF21, CPG21, Cer22, CMD⁺²², ĆPP⁺²², CTBB20, DRBT24, DZL⁺²⁰, DC22b, DOT22, FB20, FKT21, GRBN21, GD23, GX20, HM21, HCS⁺²⁰, HNCL24, HLV⁺²⁴, IW24, JK21, KZJ21, KWYN23, KS21, KdILC22, LGM20, LGM22, LYX⁺²², LSC24, MWK⁺²⁰, MNH21, MLB⁺²³, MIP⁺²², MR21, MPR22, MMF⁺²⁴, MFS22, MKB⁺²¹, MGCM21, MH20, MSS20, NHFS21, NTK21, NEG⁺²⁰, OE20, OMC⁺²⁰, OAN⁺²³, RGGD21, RB24, SDK20, SWF⁺²⁰, Sán20, dASRHB21, SC22, SMB⁺²³, SSYB⁺²⁰, SZP⁺²⁰, TANC23, TLS23, Tou21, TSH⁺²³,

VM23, WKCP21, WKL22, ZHHS21, dCVARN20, KZJ22]. **theory-based** [Ben22]. **therapeutic** [KR23]. **therapy** [ASL⁺20, DART21]. **there** [dCRM21]. **therein** [MJS⁺23, MC24]. **Thermal** [GK24, KTM⁺23, GGK20, LGJF22]. **thermally** [LYX⁺22]. **Thermochemical** [WKCP21, SSYB⁺20]. **Thermochemistry** [MHA⁺23, DKB23, OM23, RMJ21]. **Thermodynamic** [DBE20, SZLD20, CCHS23, KCGK20, MAM⁺23]. **Thermodynamics** [SK20]. **thermoelectric** [AQRA⁺23, AQMM⁺23, ABAQ⁺23, LM24, SS24]. **ThermoML** [RTB⁺22]. **thermophilic** [NYM22]. **thermophysical** [AQIS⁺24]. **Thermostabilization** [NYM22]. **ThetaPhi** [TPD21]. **thiocyanate** [SNK24b]. **Thioflavin** [Sts20]. **thioformaldehyde** [SVTK⁺22]. **thioguanine** [NST⁺20]. **thiol** [CCZ23]. **Thiols** [AWID⁺20]. **thione** [KGD⁺21, NST⁺20]. **thione-containing** [NST⁺20]. **thiophenols** [CGMRVBAI22]. **third** [GKO⁺22]. **third-neighbor** [GKO⁺22]. **those** [LML⁺23]. **Three** [PLP⁺20, KWMPR24b, LLZ⁺23, LSC⁺23, MP23, NYM22, YAO20]. **three-body** [KWMPR24b, LLZ⁺23]. **three-dimensional** [YAO20]. **three-helix** [NYM22]. **Three-site** [PLP⁺20]. **throughput** [LCP24, MZ21, NBE⁺23]. **thymine** [SSS⁺20a]. **Ti** [AQMM⁺23]. **tight** [GH22a, IYI⁺20, MCP23, NBE⁺23, NN20, Pil20, RLHG⁺23, WKCP21]. **tight-binding** [IYI⁺20, NBE⁺23, NN20, RLHG⁺23]. **Time** [BA22, YXGZ20, ABNG22, CPG21, CCPR24, FB20, HAC⁺23b, IYI⁺20, KSRB⁺21, KdILC22, LSC⁺23, MKK⁺22, MFS22, MSS20, Nan24, OMC⁺20, OAN⁺23, POvG21, TANC23]. **Time-Dependent** [YXGZ20, BA22, CPG21, FB20, IYI⁺20, MFS22, MSS20, Nan24, OMC⁺20, OAN⁺23, TANC23]. **time-evolution** [CCPR24]. **time-invariant** [KSRB⁺21]. **time-resolved** [ABNG22]. **timescale** [DWSX20]. **tiny** [ZWY⁺22]. **TiO** [IL24, VTdlM20]. **TITAN** [SHM⁺20]. **titanate** [KGG21]. **titania** [BWS20]. **titanium** [CMD⁺22]. **titrations** [WdGG24]. **TI** [ABAQ⁺23, Sai23, THH⁺24]. **TIAgF** [AQIS⁺24]. **TITaO** [LM24]. **TM** [LXP⁺22, LZW⁺23, LXP⁺22]. **TM-** [LZW⁺23]. **TMEM16** [KCF⁺20]. **Tool** [dSBFdAJ20, AAID22, ARR22b, FPMD23, GLC⁺22, LKM20, RB22, WRVP22, ZK23, ZGZC20]. **Toolkit** [PAF⁺20, AÅFJ21, CLTMd⁺23, MPP23]. **Topological** [EK20c, AA20, EPT21, HBT⁺20]. **topology** [Che23, CP23, KFLP21, MPP23, MVP⁺20, PHS⁺20, PDP⁺24, Pil20]. **torsional** [GKO⁺22]. **Total** [HTTT23]. **toughness** [MMAZ⁺23]. **toxicity** [CSG⁺21, SEBE21]. **tracking** [BBB⁺23]. **Training** [PSW⁺24]. **trajectories** [AKR21, LA20]. **Trajectory** [OSHT20, YXGZ20, FCPG20, SWLC22, ZGZC20]. **transamination** [BBC20]. **transfer** [AST24, AIV20, BBC20, BBC⁺21a, JGdC⁺23, BOPJ⁺21a, BBBP⁺23, CPG21, ĆNF23, CCPR24, IK21, KCGK20, KWB24, KPR23, Kos22, dCB23, OMC⁺20, RCC⁺20, SSYB⁺20, dCRM21]. **Transferability** [LGM22]. **transferable** [VL22]. **transform** [YLZ⁺20]. **transformation** [BLB20, IWN24]. **transient** [ABNG22, BBL⁺22].

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Anonymous:2020:CIVk

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Anonymous:2020:CIVo

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Anonymous:2020:CIVp

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Anonymous:2020:CIVt

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Anonymous:2020:CIVv

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Anonymous:2020:CIVw

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Anonymous:2020:CIVy

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Anonymous:2020:CIVz

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Anonymous:2020:CIVba

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Anonymous:2020:CIVbb

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Anonymous:2020:CIVg

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Anonymous:2020:CIVi

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Anonymous:2020:IIa

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Anonymous:2020:IIc

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Anonymous:2020:IIe

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Anonymous:2020:IIIf

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Anonymous:2020:IIg

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Anonymous:2023:IIbf

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Anonymous:2024:IIa

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Anonymous:2024:IIb

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Anonymous:2024:IIc

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Anonymous:2024:IIId

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Anonymous:2024:IIe

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Anonymous:2024:IIIf

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