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## Title word cross-reference

$(n, n)$  [BW22a].  $(n \leq 10)$  [YOCMA23].  $1$  [Pan23].  $16$  [WMJ<sup>+</sup>22].  $1 \leq N \leq 6$  [MPOC21].  $2$  [DF22, PSM<sup>+</sup>20, SLMA21].  $20$  [Wan23].  $3$  [TT20, WKL22].  $4$  [SS20].  $4H$  [MSE<sup>+</sup>21].  $5$  [AS20, JMV21, SDK20, VTdlM20].  $7$  [MdSJ<sup>+</sup>23].  $8$  [Bal20b].  $[3 + 2]$  [SMB<sup>+</sup>23].  $+$  [APR21, CWZD20, GJL21, LR20, LEP<sup>+</sup>21, MAM<sup>+</sup>23, OM22, WSV20, YMSS23].  $-$  [Tze21, WSV20, WMJ<sup>+</sup>22].  $^1$  [ZHHS21].  $^{13}$  [MCD22, ZHHS21].  $^{19}$  [Ben22, MPV22].  $^2$  [AKN<sup>+</sup>20].  $^{2+}$  [ALA<sup>+</sup>22, HSG21, IK21, JRS20, MAKZ23, SPSH20, ZRSST20].  $^{205}$  [Sai23].  $^3$  [Mar21, TTDT20].  $^{31}$  [FBP<sup>+</sup>22].  $^3\Pi_u$  [Kop22a].  $^3\Sigma_g^-$  [Kop22a].  $^\beta$  [LL21b].  $^I$  [PAS<sup>+</sup>20].  $^{II}$  [ĆPP<sup>+</sup>22].  $^{pro}$  [PPP21].  $^1$  [Dor20].  $^{10}$  [LR20, LXP<sup>+</sup>22].  $^{12}$  [PGP<sup>+</sup>23].  $^{18}$  [PP23].  $^2$  [AQMM<sup>+</sup>23, AMM22, ABAQ<sup>+</sup>23, AR20, AWK<sup>+</sup>23, DSC20, DBE20, DLH<sup>+</sup>23, DGSB<sup>+</sup>20, FP22, FP23, GGK20, GKA<sup>+</sup>23b, KPPT21, LHC<sup>+</sup>21, LZW<sup>+</sup>23, MH20, MBBU23, MMAZ<sup>+</sup>23, MK22b, OKI<sup>+</sup>21, PTP23, RC22, SSSA23, SWF<sup>+</sup>20, SWM<sup>+</sup>20b, SVTK<sup>+</sup>22, SKKG22, SBB<sup>+</sup>22,

TTK23, TYZ20, TPZ<sup>+</sup>20, TZS<sup>+</sup>22, VTdlM20, VCRP23, WP20, WLZM20, Wan23, XLW<sup>+</sup>22, YYS20, YYZ<sup>+</sup>21, ZDBZ20]. <sub>20</sub> [LR20]. <sub>24</sub><sup>0,±1,±2</sup> [MIP<sup>+</sup>21]. <sub>27</sub><sup>q</sup> [NSKN21]. <sub>2</sub><sup>+</sup> [GJL21]. <sub>2</sub><sup>-</sup> [SLR<sup>+</sup>20]. <sub>2</sub><sup>-/0</sup> [DC22a]. <sub>3</sub> [AMM22, AWK<sup>+</sup>23, BBL<sup>+</sup>22, EK20b, EK20c, IK21, KPTT21, LLS<sup>+</sup>22b, LZW<sup>+</sup>23, OE20, PTP23, PGP<sup>+</sup>23, SVTK<sup>+</sup>22, SLR<sup>+</sup>20, SM22b, SCC<sup>+</sup>22, SL20, WLZM20, XZW<sup>+</sup>21, YMSS23, dCVARN20]. <sub>4</sub> [AMM22, KGS<sup>+</sup>22, LJW<sup>+</sup>23, MK22b, SM22b, ZXD20b, ZXD20a]. <sub>450</sub> [HYA<sup>+</sup>20]. <sub>5</sub> [GJL21, HSG21, OKI<sup>+</sup>21]. <sub>6</sub> [AQMM<sup>+</sup>23, ABAQ<sup>+</sup>23]. <sub>60</sub> [DSC20, HSG21, YLZ<sup>+</sup>22]. <sub>9</sub> [PGP<sup>+</sup>23]. <sub>a</sub> [PWW20]. <sub>N</sub> [GCP22, MPOC21, SLR<sup>+</sup>20, GPM21b, KPTT21, VTdlM20, WMJ<sup>+</sup>22, YOCMA23]. <sub>n</sub> [WMJ<sup>+</sup>22, Wan23]. <sub>n</sub><sup>-/0/+</sup> [TT20]. <sub>n</sub><sup>Q</sup> [ZDBZ20]. <sub>spiro</sub> [DK23]. <sub>x</sub> [JS21]. <sub>y</sub><sup>+</sup> [JS21]. <sub>α</sub> [CSP20, DC22b, SSS<sup>+</sup>20b]. <sub>β</sub> [AV20, BPDG21, KGD<sup>+</sup>21, ZZ23b]. <sub>·</sub> [AMM22, OE20, OE20]. <sub>···</sub> [BdLC21, KPTT21, TTT<sup>+</sup>21]. <sub>d</sub> [IK21, MSE<sup>+</sup>21]. <sub>d<sup>10</sup></sub> [PTP23]. <sub>D<sub>9h</sub></sub> [PP23]. <sub>Δ</sub> [EK20a]. <sub>η<sup>1</sup></sub> [LZW<sup>+</sup>23]. <sub>η<sup>5</sup></sub> [AS23, HSG21]. <sub>f</sub> [SCZ<sup>+</sup>21]. <sub>γ</sub> [FLT23, KZJ21]. <sub>H</sub> [MIP<sup>+</sup>22]. <sub>K<sub>a</sub></sub> [SHHH22]. <sub>λ</sub> [Ngo21]. <sub>log P</sub> [DHD21, SHH<sup>+</sup>23b]. <sub>M</sub> [SM22b]. <sub>μ</sub> [MVP<sup>+</sup>20]. <sub>μ<sub>2</sub></sub> [KBHG23]. <sub>N</sub> [DOT22, MdSJ<sup>+</sup>23, NS22, OM22, PFPD21, SHH<sup>+</sup>23b]. <sub>n = 1</sub> [MdSJ<sup>+</sup>23, TT20, VTdlM20]. <sub>n = 15</sub> [Wan23]. <sub>n = 3</sub> [WMJ<sup>+</sup>22]. <sub>p</sub> [AR20]. <sub>π</sub> [AV20, CBF<sup>+</sup>20, FDD<sup>+</sup>23, LJ20, MP23, ODL20, RTB23, Sch22a, SJZ<sup>+</sup>21, TLD<sup>+</sup>22, ZBH<sup>+</sup>23]. <sub>q = 1, 0, -1</sub> [NSKN21]. <sub>S</sub> [SVTK<sup>+</sup>22]. <sub>σ</sub> [AV20, BKM21, JGGPN21, LK22, MP23, RZS<sup>+</sup>23]. <sub>sp<sup>2</sup></sub> [IW23, NUK21]. <sub>sp<sup>3</sup></sub> [NUK21]. <sub>ΘΦ</sub> [TPD21]. <sub>U</sub> [POPGS22]. <sub>v = 1, j = 0</sub> [BBY<sup>+</sup>21]. <sub>Z</sub> [ARR22b, WHJM23].

**-1** [ZDBZ20]. **-acenes** [MdSJ<sup>+</sup>23]. **-acetato** [MVP<sup>+</sup>20]. **-alanine** [DC22b]. **-alkanes** [PFPD21]. **-aminotetrazole** [JMV21]. **-aromatic** [RTB23]. **-Based** [DBE20]. **-block** [AR20]. **-bridged** [KBHG23]. **-C** [HSG21, LZW<sup>+</sup>23]. **-catalyzed** [HCY<sup>+</sup>22, LLS<sup>+</sup>22b]. **-complexes** [BKM21]. **-conjugated** [CBF<sup>+</sup>20]. **-covalency** [ZBH<sup>+</sup>23]. **-Cp** [HSG21]. **-cube** [Bal20b]. **-cyclopenta** [MSE<sup>+</sup>21]. **-dependent** [Ngo21, JRS20]. **-diaqua** [MVP<sup>+</sup>20]. **-diketones** [AV20]. **-elimination** [KZJ21]. **-F12** [CK22]. **-functions** [SCZ<sup>+</sup>21]. **-grasp** [BPDG21]. **-hairpin** [ZZ23b]. **-helical** [SSS<sup>+</sup>20b]. **-hexane** [NS22]. **-Hole** [RZS<sup>+</sup>23, JGGPN21, LK22, Sch22a, SJZ<sup>+</sup>21]. **-iron-N** [GKA<sup>+</sup>23b]. **[?]KohnEhlert:2020:PPP**. **-lactamase** [KGD<sup>+</sup>21]. **-LIO** [SDK20]. **-matrix** [WHJM23]. **-methylide** [SVTK<sup>+</sup>22]. **-modified** [DOT22]. **-octanol-water** [SHH<sup>+</sup>23b]. **-phenyl** [AS20]. **-pyrazine-M** [MH20]. **-pyrido** [MIP<sup>+</sup>22]. **-pyrrolylenones** [ARR22b]. **-radical** [MP23]. **-sextet** [TLD<sup>+</sup>22]. **-thymine** [SSS<sup>+</sup>20a]. **-water** [VCRP23]. **-xTB** [OM22].

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

**1** [CM20b, KUNT20, PWX<sup>+</sup>20, Sán20, WCT<sup>+</sup>23]. **1-11** [ZDBZ20]. **1.0**

[XSP<sup>+</sup>23]. **1.2-a** [MIP<sup>+</sup>22]. **10.1002/jcc.25747** [MT20a]. **12** [SMH21]. **19** [SLMA21].

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

**3** [GSJ<sup>+</sup>23]. **3-cycloaddition** [SVTK<sup>+</sup>22]. **3-D** [GSJ<sup>+</sup>23]. **3-trifluoro-1-nitroprop-1-ene** [SMB<sup>+</sup>23]. **3D** [CKH23, DF22, HKFT21, POPGS22, YIO20, YYZ<sup>+</sup>21]. **3D-COF** [YYZ<sup>+</sup>21]. **3D-QSAR** [DF22, HKFT21]. **3D-QSAR/MD** [HKFT21]. **3D-RISM** [CKH23, YIO20].

**4-oxo-4** [MIP<sup>+</sup>22]. **4-triazole-3-thione** [KGD<sup>+</sup>21]. **40** [MT20a]. **42** [WG21]. **43** [SCCZ21].

**6-hydroxyquinolinone** [SEBE21]. **6-lutidine** [TYZ20]. **60th** [IBL20]. **66** [FP23].

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

**8-hydroxyquinolinato** [AS20].

= [AQMM<sup>+</sup>23, ABAQ<sup>+</sup>23, AS20, APR21, GPM21b, HSG21, LZW<sup>+</sup>23, LXP<sup>+</sup>22, LJW<sup>+</sup>23, MH20, PTP23, PP23, SM22b, SCC<sup>+</sup>22, SL20, ZDBZ20].

**AA** [ZWY<sup>+</sup>22]. **Ab-initio** [RZS<sup>+</sup>23, RPD<sup>+</sup>20a, SNN<sup>+</sup>21, XSP<sup>+</sup>23]. **ABCG2** [SHH<sup>+</sup>23a]. **ABEEM** [LRqG<sup>+</sup>22]. **Absolute** [SZLD20, CV22]. **Absorption** [AS20, AS21, ABNG22, BBL<sup>+</sup>22, EK20a]. **Ac** [LJW<sup>+</sup>23]. **accelerated** [GVJ<sup>+</sup>22, PPV<sup>+</sup>21, RGGD21]. **accelerates** [NAN<sup>+</sup>23]. **Accelerating** [GCL<sup>+</sup>20, LGC21, WKL22, ABTM22]. **Acceleration** [JKS23]. **acceptor** [PTP23, TANC23]. **Accessible** [GCL<sup>+</sup>20, VCL20]. **accuracy** [RMJ21, YFH<sup>+</sup>21]. **Accurate** [DKB23, Dor20, LRF<sup>+</sup>21, PWX<sup>+</sup>20, Ben22, BP22, CSWW20, SHH<sup>+</sup>23b, SHH<sup>+</sup>23a, WD20]. **ACE2** [KLZ<sup>+</sup>23]. **acenes** [MdSJ<sup>+</sup>23]. **acetaldehyde** [LLS<sup>+</sup>22b]. **acetate2** [MIP<sup>+</sup>22]. **acetate2-oxo-2-** [MIP<sup>+</sup>22]. **acetato** [MVP<sup>+</sup>20]. **acetone** [SHHH22]. **acetonitrile** [PT21]. **acetylcholine** [BRNB21]. **Acetylene** [OOY20, SVTK<sup>+</sup>22, ZMH<sup>+</sup>21]. **achirality** [PFP<sup>+</sup>21]. **acid** [Brz22, CMD<sup>+</sup>22, FP23, HREvdK<sup>+</sup>20, HPG20, KZJ21, KK22a, KEK23, NMMC21, ODL20, OE20, PRH20, PLZT23, SHHH22, WGKG20]. **acid-catalyzed** [PRH20]. **acid-water** [KEK23]. **acidic**

[FM21, KSS21b, KSRB<sup>+21</sup>]. **acidities** [Brz22]. **acidity** [PT21]. **acids** [CH23, PT21]. **acrylate** [MSA22a]. **actinide** [SDK20]. **Actinium** [TLS23]. **actinoids** [LJW<sup>+23</sup>]. **action** [SVDS21]. **Activated** [WLZM20, LYX<sup>+22</sup>]. **Activation** [BWM20, MKSS20, MGCM21, SLR<sup>+20</sup>, ABZ20b, DZL<sup>+20</sup>, FP22, KJV23, LA20, PRF20, SHP<sup>+23</sup>]. **Active** [VDK<sup>+20</sup>, BBC20, BP22, HL20, RvWH23, TIK21, TZS<sup>+22</sup>, WS21]. **activities** [YFS20]. **activity** [BHR<sup>+21</sup>, NAAP21, SS20, DMTR22, ZMH<sup>+21</sup>]. **Acylation** [CD20]. **Ad** [FBP<sup>+22</sup>]. **Ad-MD** [FBP<sup>+22</sup>]. **adamantane** [SAZ<sup>+23</sup>]. **adamantane-like** [SAZ<sup>+23</sup>]. **adapted** [GH22b, NTK21, OE20]. **Adaptive** [SS23, NSRK21]. **Adatom** [JGSA22]. **additive** [KYM20]. **additivity** [PB20]. **adiabaticity** [RCC<sup>+20</sup>]. **adjusted** [GH22a, VV20b]. **adsorbates** [KPDB22]. **Adsorption** [GGK20, FP22, FBM<sup>+23</sup>, JGSA22, SS23, YYZ<sup>+21</sup>]. **advance** [SDH23]. **Advances** [MR21, MPR22]. **Advancing** [YGG<sup>+23</sup>]. **advantage** [BPDG21]. **aeruginosa** [VDK<sup>+20</sup>]. **affinities** [PWX<sup>+20</sup>]. **Affinity** [dSBFdAJ20, DC22b, KZOV23, NAN<sup>+23</sup>, Ngo21, NGD22, SW21, TWT<sup>+22</sup>]. **affinity-selected** [KZOV23]. **affordable** [DKB23]. **Ag** [MH20, DA22, LZW<sup>+23</sup>, PP23]. **against** [EIT<sup>+21</sup>, SKL23, UAC<sup>+23</sup>]. **agent** [SDK20]. **agents** [MML<sup>+23</sup>]. **aggregate** [RDS<sup>+20</sup>]. **aggregates** [TMO<sup>+21</sup>]. **Aggregation** [DB23]. **agonist** [BRNB21]. **aided** [KGS<sup>+22</sup>]. **AI** [AS20]. **alanine** [DC22b, FP23]. **albicans** [ZOD<sup>+22</sup>]. **Alchemical** [TM20, WFBB22, BF22, GFRNC21, HB21, Min20]. **alcohols** [ZWY<sup>+22</sup>]. **Alder** [MNZGO<sup>+20</sup>, MGCM21, NMCM21, SSYB<sup>+20</sup>]. **aldimines** [BSR22]. **aldol** [LLS<sup>+22b</sup>]. **AlGDock** [Min20]. **algebra** [GJMPVR<sup>+20</sup>]. **algebraic** [HD21]. **Algorithm** [AiIS<sup>+21</sup>, WSL<sup>+20</sup>, FR21, GKO<sup>+22</sup>, JKK<sup>+21</sup>, KG23, LHH<sup>+23</sup>, MB21, PSB<sup>+22</sup>, RD23, SS20]. **algorithms** [CP23, GWN21, POvG21, RDB23, ZKJ<sup>+23</sup>]. **alignment** [SCC<sup>+22</sup>]. **alkali** [JMV21, ODL20, OM23, OSM20, YMSS23]. **alkali-metal-like** [YMSS23]. **alkaline** [ZLLL22]. **alkanes** [PFPD21]. **alkylated** [MAP<sup>+20</sup>]. **alkylpyrroles** [ZHHS21]. **Alkyne** [WLZM20]. **Alkynes** [JFZ<sup>+20</sup>, TYZ20]. **All-atom** [PDC23, BUNO22b, LKM20, WGKG20]. **All-electron** [RNP20]. **all-metal** [MAI22]. **all-purpose** [Mar21]. **Allosteric** [BSL20, CDCT21]. **alloy** [RDB23]. **along** [CG20, MH22]. **alpha** [PFPD21]. **alpha-amylase** [PFPD21]. **alternative** [KSRKS21]. **Aluminabenzene** [Brz23]. **Aluminabenzene-based** [Brz23]. **aluminum** [BA22, Kop22a]. **AMgF** [SL20]. **amide** [CRT<sup>+21</sup>]. **amination** [DPY<sup>+22</sup>]. **amine** [CRT<sup>+21</sup>, HPG20]. **amino** [CH23, HREvdK<sup>+20</sup>, ODL20]. **aminoborane** [SR23]. **aminotetrazole** [JMV21]. **aminotransferase** [BBC20]. **AMK Mountain** [ZLLL22]. **Ammonia** [MFC20, SPSH20, YOCMA23]. **ammonium** [ODL20]. **AMOEBa** [ALA<sup>+22</sup>, PLP<sup>+20</sup>, WLWR22]. **among** [DWSX20, GFRNC21, KLZ<sup>+23</sup>]. **Amorphous** [XZZ<sup>+20</sup>, HUUO23]. **amylase** [PFPD21]. **amyloid** [BVC<sup>+23</sup>]. **analogs** [PLZT23, ZS22]. **analogues** [SJZ<sup>+21</sup>]. **Analyses** [SLR<sup>+20</sup>, AK20, GM22, GKA<sup>+23b</sup>, KZOV23, PL22, TS21]. **Analysis**

[AKR21, AD20, BBSFA22, KUNT20, MAM21, MAI22, MH20, AÅFJ21, BPL<sup>+</sup>22, BdLC21, CJHW21, CSP20, CB20, DGM22, DPY<sup>+</sup>22, ETT21b, EK20c, EPT21, HL20, HS23, IMT<sup>+</sup>21, JMK<sup>+</sup>20, JRS20, KM22, LHG<sup>+</sup>23, MDO<sup>+</sup>20, MGCM21, MT20b, NUK21, NHFS21, NTK21, NEG<sup>+</sup>20, NVBG23, OKK22, RLHG<sup>+</sup>23, RCC<sup>+</sup>20, RA20, SK23, SR23, SPT21, SWLC22, SH23, TSZ<sup>+</sup>21, YIO20, YWGY22, ZGZC20, ZBH<sup>+</sup>23]. **analytic** [BSF20, IN23b]. **Analytical** [IN23a, LL21b, VCL20]. **Analyze** [dSBFdAJ20, MPOC21, ZK23]. **analyzing** [HPG20]. **Anatomy** [LT23]. **angle** [PDL<sup>+</sup>21]. **angular** [MR21]. **anharmionic** [ETT21b]. **ANI** [TTK23]. **ANI-ML** [TTK23]. **aniline** [HRTSS<sup>+</sup>20]. **Anion** [LJ20, FDD<sup>+</sup>23, GP21, XAD20]. **anion-** [FDD<sup>+</sup>23]. **Anion-Ring** [LJ20]. **Anionic** [AK20, PT20, KPKS23]. **anions** [Brz23, GJL21, Tze21]. **Anisotropic** [GWN21, ZGZ<sup>+</sup>20, AYO20, BS23]. **anisotropy** [SSP23]. **annulene** [PC21]. **AnO** [LJW<sup>+</sup>23]. **anode** [SGT<sup>+</sup>20]. **anomaly** [XCJ20]. **antagonists** [CM20b]. **anthracene** [MNZGO<sup>+</sup>20]. **Anti** [KUNT20, NPGP23, SVDS21]. **anti-cancer** [SVDS21]. **anti-HIV** [NPGP23]. **Anti-Human** [KUNT20]. **antibiotic** [BF22]. **Antibodies** [KUNT20]. **anticancer** [HBM<sup>+</sup>20]. **antiferromagnetic** [Wan23]. **antimicrobial** [SEBE21]. **antimony** [PT21]. **antiporter** [WSV20]. **antipsychotic** [dCRM21]. **antitumor** [PRH20]. **any** [dCRM21]. **applicability** [GH22a, LSP23]. **Application** [GJMPPB<sup>+</sup>20, KdILC22, MZ21, PHS<sup>+</sup>20, TM20, Tou21, XAD20, AAe20, MLC<sup>+</sup>23, MK22b, SS23, TSR21, YLZ<sup>+</sup>20, YBS<sup>+</sup>20]. **Applications** [BBC<sup>+</sup>21a, SHM<sup>+</sup>20, AQMM<sup>+</sup>23, CC22, IYI<sup>+</sup>20, IRB<sup>+</sup>23, KGS<sup>+</sup>21, SIW21, SKS21, SPT21, TCS<sup>+</sup>21a]. **applied** [HBM<sup>+</sup>20, KCGK20, PMT<sup>+</sup>22]. **apply** [PDL<sup>+</sup>21]. **Approach** [PWW20, SBG20, SB20, ARR22a, ARR22b, AAL21, ASW20, CN21, ĆPP<sup>+</sup>22, DGSB<sup>+</sup>20, DOT22, HBT<sup>+</sup>20, IYI<sup>+</sup>20, IRB<sup>+</sup>23, JGGPN21, KG23, KPHV23, KEK23, LBH<sup>+</sup>22, LL22, LDT<sup>+</sup>22, MZMK<sup>+</sup>21, MJS<sup>+</sup>23, MSA22b, NMFI21, OSHT20, PW20, RDB23, STR20, TAC<sup>+</sup>23, TMO<sup>+</sup>21, TSR21, VCL20, YC23]. **approaches** [AV20, GH22a]. **approximate** [BSS<sup>+</sup>22, JCMHT22]. **approximation** [BMT<sup>+</sup>21, CS23, MCP23, NG20, Shi22, VV20b, YW20]. **Approximations** [HFPS20, BSF20, RC22]. **aprotic** [OM22]. **aptamer** [KR23, TM20]. **AQUA** [LGD<sup>+</sup>20]. **AQUA-MER** [LGD<sup>+</sup>20]. **aquation** [HBM<sup>+</sup>20]. **Aqueous** [SSYB<sup>+</sup>20, KK23, KTM<sup>+</sup>23, LGD<sup>+</sup>20, PDC23, RPD<sup>+</sup>20a, VV21, YC20]. **Archive** [RTB<sup>+</sup>22]. **Area** [GCL<sup>+</sup>20, VCL20]. **Arene** [KGS<sup>+</sup>21]. **Argentophillic** [EPT21]. **argentum** [EPT21]. **argon** [NSH23]. **ARGOS** [NSRK21]. **arithmetic** [LPF<sup>+</sup>23]. **ArN** [MAM<sup>+</sup>23]. **aromatic** [APS20, GAP21, MAI22, ODL20, RTB23, TLD<sup>+</sup>22]. **art** [BSF20]. **artifacts** [ÖLP<sup>+</sup>20]. **Artificial** [QB20, MZ21]. **aryne** [GM22]. **Aspartate** [HPG20, BBC20]. **aspects** [KZJ22]. **asplatin** [PPSP20]. **assemblies** [GBM20]. **assembly** [MAP<sup>+</sup>20, PRH20]. **Assessing** [BOPJ<sup>+</sup>21a, PRF20, MK22a]. **Assessment** [AS21, CK22, FB21, POPGS22, RC22, SK20, SB20, ZRSST20]. **assisted**

[ARA22, AV20, ARR22b, CRT<sup>+</sup>21, HUO23, KGTL21, LL21b, LL22, MLC<sup>+</sup>23, WRBT21]. **association** [GBM20, SSS<sup>+</sup>20b, YJZ<sup>+</sup>22]. **astatine** [PHS<sup>+</sup>20]. **asymmetric** [HCY<sup>+</sup>22]. **atom** [BUNO22b, DART21, DLH<sup>+</sup>23, GFRNC21, LKM20, LK22, PDC23, SHH<sup>+</sup>23a, WMJ<sup>+</sup>22, WGKG20]. **atom-centered** [LK22]. **atomic** [AÁFJ21, BP22, EVKL21, LL21b, NEG<sup>+</sup>20]. **atomicity** [NAAP21]. **Atomistic** [GOY20, HZG<sup>+</sup>20, ONA<sup>+</sup>20, SY21, SL20, WKD<sup>+</sup>21, FLT23, LGC21, RMS<sup>+</sup>23]. **atomistically** [NP23]. **atomization** [GZFSM21, MCP23]. **atoms** [AKN<sup>+</sup>20, AA20, CC22, CSGVF<sup>+</sup>20, DC22a, JCMHT22, JGGPN21, LGM20, LGM22, LYX<sup>+</sup>22, MSYS23, MC23, NTK21, NSH23, OE20, Sch22b, SG20, Wan23]. **atoms-in-molecules** [MC23, NTK21]. **attack** [CRT<sup>+</sup>21]. **attraction** [IN23b]. **attractors** [KE23b]. **augmented** [NEG<sup>+</sup>20, Pil20]. **auto** [CJHW21]. **auto-analysis** [CJHW21]. **AutoDock** [PNT<sup>+</sup>22]. **Automated** [COK22, GSD<sup>+</sup>22, WHJM23, ZLLL22, MNBG<sup>+</sup>21, RSHG23, RB22, SSMP23]. **Automatic** [SM22a, FKT21]. **Automation** [WLWR22]. **Automotive** [SC23]. **Automatized** [ABNG22, SYS<sup>+</sup>21]. **AutoMeKin2021** [MNBG<sup>+</sup>21]. **auxetic** [MMAZ<sup>+</sup>23]. **auxiliary** [MFS22, NSH23, SM22a]. **available** [TPD21]. **averaged** [TWT<sup>+</sup>22]. **Avoids** [SZLD20]. **aware** [TCS<sup>+</sup>21a]. **axial** [GSJ<sup>+</sup>23, PPFL23]. **Aza-BODIPY** [FB21]. **azabenzenes** [BKM21]. **azide** [XZZ<sup>+</sup>20]. **Azobenzene** [YXGZ20, YLZ<sup>+</sup>22]. **azobenzene-containing** [YLZ<sup>+</sup>22]. **AzoChignolin** [ZZ23b]. **azomethine** [SMB<sup>+</sup>23].

**B** [LHC<sup>+</sup>21, PGP<sup>+</sup>23, YMSS23, DZL<sup>+</sup>20, DDSM23, MIP<sup>+</sup>21]. **B3LYP** [LRF<sup>+</sup>21, SW21]. **Back** [KE23a, GAG20]. **Backbone** [CLS<sup>+</sup>20, OC23, SGGG22, SSS<sup>+</sup>20b, LL21b]. **backbone-driven** [SSS<sup>+</sup>20b]. **balance** [LBH<sup>+</sup>22, SSS<sup>+</sup>20b]. **balanced** [BK22]. **band** [GAP21, MA23a, MA23b, ZLLL22, LPP20]. **bandgap** [dARW<sup>+</sup>23]. **bands** [Sch22a]. **BAR** [ZK21]. **barriers** [MML<sup>+</sup>23]. **Barshad** [VFCG20]. **base** [DDSM23]. **Based** [DBE20, AV20, ARR22a, BAO<sup>+</sup>20, Ben22, Brz23, CDCT21, CM20a, CP23, CN21, DC22b, DPY<sup>+</sup>22, DGSB<sup>+</sup>20, EK20a, FP22, FKT21, GJMPVR<sup>+</sup>20, GJMPB<sup>+</sup>20, GRBN21, GLC<sup>+</sup>22, HM21, JMV21, KWYN23, KGS<sup>+</sup>21, KZOV23, KDKS21, KdILC22, KSRKS21, KDP<sup>+</sup>22, LHH<sup>+</sup>21, LSP23, LWF<sup>+</sup>22, LEP<sup>+</sup>21, LC22, MNZGO<sup>+</sup>20, MKK<sup>+</sup>22, MLG<sup>+</sup>21b, MAKZ23, MT20b, NEG<sup>+</sup>20, OE20, PPV<sup>+</sup>21, PW20, PMT<sup>+</sup>22, PM21, RKC21, RDK<sup>+</sup>22, RSHG23, RCC<sup>+</sup>20, RDB23, SKL23, SBB<sup>+</sup>22, SM20, SD21, SHHH22, TWT<sup>+</sup>22, UB20, VWP<sup>+</sup>22, Vyb23, YLZ<sup>+</sup>20, ZLLL22, ZS22, ZFRM20]. **bases** [Sch22a]. **basicity** [DC22b, GSH23, SW21]. **Basis** [YXGZ20, CM20b, GZFSM21, GH22b, IN23b, LB21, LB22, MFS22, MCP23, NSH23, RNP20, SLB23, SM22a, SCKH21, SM20, SCCZ21, TAC<sup>+</sup>23, WCT<sup>+</sup>23]. **basis-set** [TAC<sup>+</sup>23]. **bath** [CQSG20]. **batteries** [SGT<sup>+</sup>20]. **Bayesian** [AVM21, LBH<sup>+</sup>22]. **Bdf1** [ZOD<sup>+</sup>22]. **Be** [ZDBZ20, BTSB22, SKKG22, YOCMA23, YMSS23]. **BeH** [MMAZ<sup>+</sup>23]. **Behavior** [NI22, AK20, KDKS21]. **Bel** [ZXD20b, ZXD20a]. **BeM** [PTP23].

**Benchmark** [DC22b, MLP22, SW21, SC22, AZKM22, CPG21, CS20, DGSB<sup>+20</sup>, NAN<sup>+23</sup>, OMC<sup>+20</sup>, dASRHB21]. **Benchmarking** [LSP23, MAKZ23, XZ20, RLHG<sup>+23</sup>, SI22]. **beneficial** [BTSB22]. **Benoit** [IBL20]. **bent** [WG20]. **benzaldehyde** [DSK21, NMMC21, SW21]. **benzene** [NMF121, RC22, XCJ20, ZS22]. **benzene-bridged** [ZS22]. **benzoin** [DSB23]. **benzyne** [GM22]. **benzyne/aryne** [GM22]. **Beryllium** [MSYS23, Kop22b, PTP23, RMS<sup>+23</sup>, SKKG22, THLC<sup>+23</sup>, ZDBZ20]. **beryllium-doped** [ZDBZ20]. **best** [KDP<sup>+22</sup>, ZHHS21]. **between** [BW22a, CS20, CTBB20, dSCCN21, HYA<sup>+20</sup>, KR23, Klo22, KPR23, MML<sup>+23</sup>, MPP23, Min20, NTK21, PTP23, RZS<sup>+23</sup>, SMB<sup>+23</sup>, SSS<sup>+20b</sup>]. **BFGS** [FR21]. **bias** [KSRB<sup>+21</sup>, Tik23]. **biased** [DHN<sup>+21</sup>, RGGD21]. **biased/accelerated** [RGGD21]. **biasing** [GVJ<sup>+22</sup>, RR22]. **bidentate** [LLKS23, TLS23]. **bidirectional** [MPP23, MMAZ<sup>+23</sup>]. **bifunctional** [HBM<sup>+20</sup>]. **bile** [WGKG20]. **bileptic** [GPM21b]. **bimetallic** [MAKZ23]. **binary** [MJS<sup>+23</sup>]. **BinderSpace** [KZOV23]. **Binding** [GOY20, KLZ<sup>+23</sup>, KPKS23, MXM20, Min20, NNT<sup>+20</sup>, SZLD20, dSBFdAJ20, BRNB21, CSP20, FDD<sup>+23</sup>, GH22a, HGF20, IYI<sup>+20</sup>, KR23, MAKZ23, MSA22a, NAN<sup>+23</sup>, NTK21, NBE<sup>+23</sup>, Ngo21, NST<sup>+20</sup>, NGD22, NN20, ÖLP<sup>+20</sup>, PWX<sup>+20</sup>, RLHG<sup>+23</sup>, SWF<sup>+20</sup>, SWM<sup>+20b</sup>, SSO<sup>+20</sup>, TWT<sup>+22</sup>, WKCP21, XZX<sup>+22</sup>, YIO20, ZOD<sup>+22</sup>]. **binuclear** [KKAK23]. **bio** [AAID22]. **bio-membranes** [AAID22]. **bioactivity** [MPuS<sup>+20</sup>]. **biochemical** [YWGY22]. **Biological** [AWID<sup>+20</sup>, CKH23, CBB<sup>+21</sup>, JKK<sup>+21</sup>, JKS23, SS20]. **biology** [FPMD23, IBL20]. **biomacromolecules** [LRKD23]. **biomolecular** [MAKZ23]. **Biomolecules** [WZZ<sup>+20</sup>, SH23, ZGZC20]. **biophysical** [SKS21]. **bioremediation** [PFPD21]. **biosensor** [SPT21]. **biosystems** [GUCCR20]. **biphenyl** [BdLC21]. **biphenylene** [RTB23]. **BIPS** [DK23]. **birthday** [IBL20]. **bis** [YFS20]. **Block** [RA20, AR20, LRKD23]. **blocks** [RA20]. **Blue** [HBM<sup>+20</sup>]. **BMP** [CM20b]. **BMP-2** [CM20b]. **BMP-7** [CM20b]. **BN** [MdSJ<sup>+23</sup>]. **BN-** [MdSJ<sup>+23</sup>]. **BODIPY** [FB21]. **BODIPY/Aza** [FB21]. **BODIPY/Aza-BODIPY** [FB21]. **body** [BMT23, KG23, KSP21, LLZ<sup>+23</sup>, NI22, VWJ23, WFLZ23]. **Bohmian** [Tik23]. **Bohmian-style** [Tik23]. **Boltzmann** [NSRK21, RCC21, SCvW22, WK21, XAD20]. **Bond** [LR20, AV20, ARR22b, AD23, APR21, BKM21, CRT<sup>+21</sup>, DK23, GH22a, HL20, HSG21, MDO<sup>+20</sup>, MLB<sup>+23</sup>, MIP<sup>+22</sup>, MC23, PDL<sup>+21</sup>, Sch22b, SSS<sup>+20a</sup>, SJZ<sup>+21</sup>, SHP<sup>+23</sup>, TTT<sup>+21</sup>, XCJ20, ZMH<sup>+21</sup>]. **bond-angle** [PDL<sup>+21</sup>]. **bonded** [DGM22, LKT21, LML<sup>+23</sup>]. **Bonding** [DDSM23, FNP22, GM22, KE23b, LHG<sup>+23</sup>, MCD22, SMH21, THLC<sup>+23</sup>, AV20, AWK<sup>+23</sup>, AA20, BGS<sup>+20</sup>, BCN22, CVGVN<sup>+20</sup>, DGM22, EK20c, FDK22, GKA<sup>+23b</sup>, GSJ<sup>+23</sup>, JC20, JGGPN21, LLKS23, LXP<sup>+22</sup>, MVP<sup>+20</sup>, MSYS23, MP23, MIP<sup>+21</sup>, NEG<sup>+20</sup>, Tze21, WCD<sup>+23</sup>, ZBH<sup>+23</sup>, dBcDL20]. **bonds** [Brz22, CB20, GH22a, HS23, KPTT21, NTK21, PTP23, SGGG22, dASRHB21, Sch22b, SD21, WG20, ZBH<sup>+23</sup>]. **Boosting** [KN21]. **borane**

[ZZG<sup>+</sup>21]. **boranylborane** [PFP<sup>+</sup>21]. **Born** [GCL<sup>+</sup>20]. **Boron** [FP22, MAI22, ZS22]. **boron/phosphorus** [ZS22]. **boron/phosphorus-based** [ZS22]. **boronic** [FP23]. **borylene** [DGM22]. **both** [KCF<sup>+</sup>20, PRH20]. **boundary** [CX21b, PSMPB21, RCC21, SCvW22, YAO20]. **bpy** [IK21]. **Br** [SCC<sup>+</sup>22, ABAQ<sup>+</sup>23, GGK20, MBBU23]. **Branched** [TPB22]. **breakage** [FVSS20]. **Breakdown** [AD20]. **Breaking** [LR20]. **breathing** [CBF<sup>+</sup>20]. **Breit** [IN23a]. **Breslow** [DSB23]. **brevicompactum** [HYA<sup>+</sup>20]. **bridged** [KBHG23, ZS22]. **Bridging** [HZG<sup>+</sup>20, LLKS23]. **Brownian** [LL21a, Shi22]. **Brownian-type** [LL21a]. **BSSE** [LB21, LB22, SLB23]. **BSSE-corrected** [LB21, LB22, SLB23]. **buckle** [GNL<sup>+</sup>22]. **buckybowls** [FDD<sup>+</sup>23]. **buffer** [FKT21]. **Building** [AD20, AAID22, LRKD23]. **building-block** [LRKD23]. **bulk** [CX21b, TANC23, dARW<sup>+</sup>23]. **bundle** [NYM22, SIW21].

**C** [GPM21b, HSG21, LR20, LZW<sup>+</sup>23, OKI<sup>+</sup>21, PP23, ZFRM20, ARR22b, DZL<sup>+</sup>20, DSC20, DK23, GAP21, MPuS<sup>+</sup>20, MCP23, MCD22, PGP<sup>+</sup>23, SHP<sup>+</sup>23, YLZ<sup>+</sup>22, ZHHS21]. **C-NMR** [MCD22]. **C2** [FCB23]. **C22** [FCB23]. **cAAC** [GPM21b]. **Cage** [SSSA23, DSC20, GGK20]. **Cage-size** [SSSA23]. **CAI** [ZXD20a]. **CAI** [ZXD20b]. **calculate** [FBP<sup>+</sup>22, SS20, WFBB22]. **calculated** [ABAQ<sup>+</sup>23]. **Calculation** [CV22, Sán20, CSWW20, KM22, MR21, NML21, ÖLP<sup>+</sup>20, PRF20, SCCZ21, VCL20, VV21, YBS<sup>+</sup>20]. **Calculations** [DBE20, MXM20, Min20, AiIS<sup>+</sup>21, BSS<sup>+</sup>22, BSR22, CKH23, CLTMd<sup>+</sup>23, DGsb<sup>+</sup>20, EK20b, EPT21, FV20, FB20, GBM20, HB21, HM21, HRTSS<sup>+</sup>20, KL20, KK23, LB21, LB22, MLC<sup>+</sup>23, MAM<sup>+</sup>23, Mar21, MCD22, NAN<sup>+</sup>23, PFSC20, QLC<sup>+</sup>20, RH21, SW21, SRB21, SWF<sup>+</sup>20, SWM<sup>+</sup>20b, SSMP23, SLB23, SZP<sup>+</sup>20, TM20, TT20]. **Calibration** [DPSG20]. **CAM** [LRF<sup>+</sup>21]. **CAM-B3LYP** [LRF<sup>+</sup>21]. **camptothecin** [PRH20]. **Can** [BTSB22, PBM21]. **cancer** [SVDS21]. **Candida** [ZOD<sup>+</sup>22]. **canonical** [GGK20, KSRB<sup>+</sup>21, ZKJ<sup>+</sup>23]. **capacity** [SKKG22]. **capture** [BBB<sup>+</sup>23, KOD21]. **carbene** [DGM22]. **carbene-borylene** [DGM22]. **Carbenes** [PAS<sup>+</sup>20, JGSA22, KJV23]. **Carbocyclic** [PAS<sup>+</sup>20]. **carbohydrates** [KB22]. **Carbon** [ZXD20a, APS20, AS21, AKN<sup>+</sup>20, BW22a, CBF<sup>+</sup>20, CTBB20, DC22a, GPEK<sup>+</sup>20, GKA<sup>+</sup>23b, IW23, LZW<sup>+</sup>23, MP23, PGP<sup>+</sup>21, RZS<sup>+</sup>23, ZSD<sup>+</sup>20, ZXD20b]. **carbonyl** [FNPD22]. **carboxy** [FDK22]. **carboxy-neuroglobin** [FDK22]. **carboxylate** [OSM20]. **carboxylate-promoted** [OSM20]. **carboxylates** [PCI23]. **carboxylation** [JMK<sup>+</sup>20]. **Carlo** [DMD<sup>+</sup>21, EG20, GGK20, GNL<sup>+</sup>22, KCGK20, KEK23, PFSC20, TIK21, TMO<sup>+</sup>21, ZKJ<sup>+</sup>23]. **Carlo/DFT** [TMO<sup>+</sup>21]. **carrier** [LHC<sup>+</sup>21, ZGZ<sup>+</sup>20]. **Cartesian** [BLB20]. **Case** [ARR22b, AA20, HM21, LWLC21, NPGP23, OSHT20, PDGD23, RPD<sup>+</sup>20a, TMO<sup>+</sup>21, VM23]. **CASPT2** [TT20]. **Cassandra** [DMD<sup>+</sup>21]. **CASSCF** [LJW<sup>+</sup>23, Sts20]. **catalysis** [JRS20]. **catalyst** [CJHW21, MAM21]. **catalysts** [DLH<sup>+</sup>23, MLB<sup>+</sup>23, MKB<sup>+</sup>21, SHP<sup>+</sup>23, WKG<sup>+</sup>23]. **catalytic** [CJHW21, CL23, DSK21, MKB<sup>+</sup>21, PFPD21, PM21, YFS20, ZMH<sup>+</sup>21].

**Catalyzed** [LLS<sup>+22b</sup>, AMM22, HCY<sup>+22</sup>, HYA<sup>+20</sup>, NMMC21, PRH20].  
**Cation** [LJ20, Kop22b, ODL20, PGP<sup>+23</sup>, YMSS23, dARW<sup>+23</sup>]. **cationic** [KPKS23]. **cations** [APR21, Jab22a]. **CATKINAS** [CJHW21]. **caused** [LML<sup>+23</sup>]. **Cavity** [GRN20, BBSFA22, MJS<sup>+23</sup>]. **CBS** [CSWW20, Dor20, SK20]. **CC3** [GGK20]. **CC3-R** [GGK20]. **CCI** [KGS<sup>+22</sup>]. **CCSD** [CS20, CK22, CSWW20, Dor20, GRBN21, KG23, MLB<sup>+23</sup>, MEKH22, MCP23, PRF20, SI22]. **CCSDT** [SK20]. **Cd** [JS21]. **CdSe** [LWLC21]. **Celebrating** [IBL20]. **cells** [AYO20, SZP<sup>+20</sup>, TANC23]. **CellSys** [AAID22]. **cellulose** [LGJF22]. **center** [LK22]. **centered** [LK22]. **CEPA/1** [Sán20]. **CGeGaAl** [DC22a]. **CH** [AMM22, SVTK<sup>+22</sup>, dCVARN20, BdLC21, KPTT21, MK22b, SVTK<sup>+22</sup>, SLR<sup>+20</sup>, SCC<sup>+22</sup>, XZW<sup>+21</sup>, dCVARN20]. **chain** [Shi22, SSS<sup>+20b</sup>]. **chains** [BSR22, ODL20]. **Chalcogen** [MDO<sup>+20</sup>, dASRHB21]. **Chalcogen-mercury** [MDO<sup>+20</sup>]. **chalcogenides** [EPT21]. **chalcogenuranes** [dSCCN21]. **chalcone** [ARR22a]. **challenge** [RLHG<sup>+23</sup>, RvWH23]. **Challenging** [JGGPN21, BOPJ<sup>+21a</sup>, CTPJH22, UB20, VM23]. **Chalmers** [AÁFJ21]. **CHAMPION** [AÁFJ21]. **change** [JGM21]. **changes** [BBSFA22, ÖLP<sup>+20</sup>, TTH<sup>+21a</sup>]. **changing** [PNT<sup>+22</sup>]. **channel** [CX21b, LA20, XAD20]. **channels** [OKI<sup>+21</sup>]. **Chaperone** [VDK<sup>+20</sup>]. **character** [BGS<sup>+20</sup>, LHG<sup>+23</sup>, SD21]. **characteristics** [KZP22, MML<sup>+23</sup>]. **Characterization** [BVC<sup>+23</sup>, PT20, dBCdL20, GPEK<sup>+20</sup>, Kop22a, LZW<sup>+23</sup>, MC23, PGP<sup>+21</sup>, SBB<sup>+22</sup>]. **characterize** [LKK<sup>+23</sup>]. **Charge** [GRN20, SKKK20, BBC<sup>+21a</sup>, BOPJ<sup>+21a</sup>, CPG21, CB20, IN23b, IK21, KCGK20, NVBG23, ÖLP<sup>+20</sup>, OMC<sup>+20</sup>, PLP<sup>+20</sup>, PWX<sup>+20</sup>, SPSH20, SK23, SZL23, SHH<sup>+23a</sup>, XZW<sup>+21</sup>, ZWY<sup>+22</sup>, ZGZ<sup>+20</sup>, dCRM21]. **charge-scaling** [ZWY<sup>+22</sup>]. **charge-transfer** [BBC<sup>+21a</sup>, BOPJ<sup>+21a</sup>, IK21]. **charged** [HPG20, SSP23]. **charges** [CX21b, LK22, NEG<sup>+20</sup>]. **Charm** [WMZJ20]. **CHARMM** [FVSS20, KLP<sup>+22</sup>, KYM20, QLC<sup>+20</sup>, TPB22, VWP<sup>+22</sup>]. **CHARMM-based** [VWP<sup>+22</sup>]. **CHARMM-GUI** [KLP<sup>+22</sup>, QLC<sup>+20</sup>]. **Chem** [MT20a, WG21, CSG<sup>+21</sup>]. **chemcoord** [WHJM23]. **Chemical** [AWK<sup>+23</sup>, AWID<sup>+20</sup>, CGMRVBAl22, DF22, MSL<sup>+20</sup>, Ooy20, PAS<sup>+20</sup>, VAL20, WG21, APR21, BHR<sup>+21</sup>, Ben22, BBK<sup>+21</sup>, CKH23, CP23, CSG<sup>+21</sup>, CB20, DGSB<sup>+20</sup>, EK20c, HGF20, KFLP21, KB22, LT23, LC22, MLC<sup>+23</sup>, MH22, MN20, MAI22, MPV22, NEG<sup>+20</sup>, OKI<sup>+21</sup>, PHS<sup>+20</sup>, Pil20, RSHG23, SBFSJMLU23, SIW21, SYS<sup>+21</sup>, SC23, SR23, SCC<sup>+22</sup>, TANC23, TTDT20, Tze21, UB20, VWJ23, Wan21a, Wan21b, WHJM23, YGG<sup>+23</sup>, ZHHS21]. **chemical-bonding** [NEG<sup>+20</sup>]. **chemically** [BUNO22b, BP22, TCS<sup>+21a</sup>]. **chemicals** [CSG<sup>+21</sup>, WRVP22]. **Chemisorption** [PKT21]. **chemistry** [BBB<sup>+23</sup>, DKB23, GP21, KRSD<sup>+23</sup>, LGM20, NVBG23, PSGL21, SDK20, SSMP23, SNN<sup>+21</sup>, TPD21, TLS23, TCS<sup>+21a</sup>, TV22, TSH<sup>+23</sup>, VAP<sup>+21</sup>, XSP<sup>+23</sup>]. **Chignolin** [ZZ23b]. **ChimeraX** [SIW21]. **chiral** [GJMPVR<sup>+20</sup>, MNZGO<sup>+20</sup>, PFP<sup>+21</sup>, SRB21]. **chirality** [PPFL23]. **chloride** [Mil21]. **choice** [SCKH21]. **Cholesterol** [Ban20]. **chromophore** [RPD<sup>+20a</sup>]. **chromophores** [BSR22, MSA22b]. **CI** [CN21, Gie21].

**CIFDock** [VWP<sup>+</sup>22]. **circular** [MSA22b]. **Cis** [YXGZ20]. **Cis-Azobenzene** [YXGZ20]. **CI** [SCC<sup>+</sup>22, ZG21, ABAQ<sup>+</sup>23, GGK20, MBBU23, SLR<sup>+</sup>20, WSV20]. **CL-20** [ZG21]. **CL-20/HMX** [ZG21]. **Clar** [TLD<sup>+</sup>22]. **classic** [MAI22]. **classical** [BdLC21, DHD21, HUUO23, KLP<sup>+</sup>22]. **ClassicalGSG** [DHD21]. **classify** [DTA21]. **clathrate** [VCRP23]. **clathrate-hydrates** [VCRP23]. **cleavage** [CRT<sup>+</sup>21, JRS20]. **close** [CGMRVBAI22]. **closed** [Klo22, MB21]. **closed-shell** [Klo22, MB21]. **Cluster** [BLP20, WZZ<sup>+</sup>20, BTSB22, BSF20, DC22b, FB21, GRBN21, HPM<sup>+</sup>21, KPDB22, NSKN21, SKKG22, SAZ<sup>+</sup>23, STR20, WP20]. **cluster-continuum** [STR20]. **Clusters** [MFC20, AD23, BWS20, CVGVN<sup>+</sup>20, DZL<sup>+</sup>20, JS21, KE23b, KPTT21, KG23, KEK23, LL21a, LLZ<sup>+</sup>23, LXP<sup>+</sup>22, MAI22, Mil21, NAAP21, NI22, NST<sup>+</sup>20, OM23, POPGS22, RDB23, TT20, TSR21, VTdIM20, WMJ<sup>+</sup>22, Wan23, YOCMA23, ZDBZ20]. **Cm** [LJW<sup>+</sup>23]. **CO** [PTP23, WLZM20, LXP<sup>+</sup>22, DZL<sup>+</sup>20, GKA<sup>+</sup>23b, MSA22a, AMM22, AR20, DGSB<sup>+</sup>20, FP22, FP23, FDK22, LHC<sup>+</sup>21, MK22b, RC22, SK23, SBB<sup>+</sup>22, VCRP23, WP20, XLW<sup>+</sup>22, YYZ<sup>+</sup>21]. **co-deposition** [MSA22a]. **co-factor** [GKA<sup>+</sup>23b]. **CO-N** [XLW<sup>+</sup>22]. **Coarse** [MT20a, WSL<sup>+</sup>20, WZZ<sup>+</sup>20, BS23, CST23, GWN21, KGTL21, LL21b, LL22, MT19, SSDL<sup>+</sup>23]. **Coarse-Grained** [MT20a, WSL<sup>+</sup>20, WZZ<sup>+</sup>20, BS23, CST23, GWN21, KGTL21, LL21b, LL22, MT19, SSDL<sup>+</sup>23]. **cobalt** [HCY<sup>+</sup>22]. **COBRAMM** [ABNG22]. **cocrystal** [ZG21]. **Code** [SHM<sup>+</sup>20, TS21]. **codelivery** [PRH20]. **codes** [WK21]. **coefficient** [SHH<sup>+</sup>23b, UKBD23]. **coefficients** [BUNO22b]. **Coelenterazine** [GOY20]. **Coenzyme** [CWZD20]. **COF** [YYZ<sup>+</sup>21]. **coherent** [EVKL21]. **coinage** [FBM<sup>+</sup>23, MCD22]. **collision** [BBY<sup>+</sup>21]. **Colorings** [Bal20a]. **combination** [GVJ<sup>+</sup>22, KK23]. **Combined** [RMJ21, AiS<sup>+</sup>21, KPHV23, LDT<sup>+</sup>22, TIK21, TMO<sup>+</sup>21, WKD<sup>+</sup>21]. **Combining** [BMT<sup>+</sup>21, MKB<sup>+</sup>21, TCS<sup>+</sup>21a, WSL<sup>+</sup>20, KN21, NML21]. **Comment** [MT21, NTK21, WFLZ23, WG21, CPG21, Wan21a]. **common** [MSA22a]. **communications** [AiS<sup>+</sup>21]. **Comparative** [JMV21, PM21]. **compared** [LML<sup>+</sup>23, WD20]. **Comparing** [CCHS23]. **Comparison** [BSS<sup>+</sup>22, CN21, NUK21, RLHG<sup>+</sup>23, SK20, WK21, DGM22, GG22, HSG21, SVTK<sup>+</sup>22, SK23]. **compatible** [PLP<sup>+</sup>20]. **competition** [SJZ<sup>+</sup>21]. **complementary** [FPMD23, SM22a]. **Complete** [HL20, DMD<sup>+</sup>21, MCP23, SCKH21]. **Complex** [NGD22, ALA20, AAL21, BF22, GNK<sup>+</sup>23, KL20, LML<sup>+</sup>23, OE20, SWF<sup>+</sup>20, SIW21, SC23, TM20, WHJM23, YYS20, ZMH<sup>+</sup>21, ZZG<sup>+</sup>21]. **complexation** [SDK20]. **Complexes** [AD20, BGS<sup>+</sup>20, ASL<sup>+</sup>20, AS23, AS20, BKM21, Brz22, CL23, CMD<sup>+</sup>22, ĆPP<sup>+</sup>22, DGM22, DSK21, FNP22, GKA<sup>+</sup>23b, GP21, Jab22a, KK23, KBHG23, KKAK23, KDP<sup>+</sup>22, LLKS23, LKT21, LZW<sup>+</sup>23, LML<sup>+</sup>23, MNH21, MVP<sup>+</sup>20, MGB<sup>+</sup>22, MCD22, NBE<sup>+</sup>23, PTP23, PB20, PP23, RLHG<sup>+</sup>23, SVDS21, SEZ20, SD21, THLC<sup>+</sup>23, XZX<sup>+</sup>22, YFS20, dBCdL20]. **component** [KWYN23, KL20]. **components** [AV20, NTK21]. **composite** [CK22, PW20].

**composites** [MML<sup>+</sup>23]. **Composition** [YLZ<sup>+</sup>22, JS21].  
**Composition-selective** [YLZ<sup>+</sup>22]. **compound**  
 [EK20b, HTFY21, QLW<sup>+</sup>22b, SWM<sup>+</sup>20b]. **compound-protein** [QLW<sup>+</sup>22b].  
**Compounds** [PAS<sup>+</sup>20, SL20, BW22a, MAI22, MCP23, MP23, NI22,  
 NPGP23, PDGD22, PDGD23, PHS<sup>+</sup>20, QLW<sup>+</sup>22b, SW21]. **Comprehensive**  
 [YIO20, PRH20, ZK23]. **compressed** [XZZ<sup>+</sup>20]. **compression** [CC22].  
**Comput** [MT20a, WG21]. **Computation**  
 [ALA20, CM20a, GZFSM21, MN20, SZL23]. **Computational**  
 [ARA22, AD20, AR20, BW22a, GOY20, KZP22, KJV23, KBHG23, MPV22,  
 Sai23, SKGG23, XZ20, ZMH<sup>+</sup>21, CRT<sup>+</sup>21, JC20, KZJ22, KPHV23, LCP21,  
 MDO<sup>+</sup>20, MK22a, MSA22b, NMMC21, PSGL21, SW21, SVDS21, SBB<sup>+</sup>22,  
 TTH<sup>+</sup>21a, VAP<sup>+</sup>21, WG20]. **Computationally** [ZBH<sup>+</sup>23, TPD21].  
**Computations** [Bal20a, Bal20b, BSF20, RBM<sup>+</sup>23]. **compute** [SYS<sup>+</sup>21].  
**computed** [MEKH22, ZWR22]. **Computer** [KGS<sup>+</sup>22]. **Computer-aided**  
 [KGS<sup>+</sup>22]. **Computing** [GJMPVR<sup>+</sup>20, IRB<sup>+</sup>23, JKK<sup>+</sup>21, MPP23, POvG21].  
**concentrations** [CX21b]. **conceptual** [ČPP<sup>+</sup>22, GD23, MGCM21].  
**concern** [KLZ<sup>+</sup>23, WRVP22]. **concerning** [VTdM20]. **concerted**  
 [SBB<sup>+</sup>22]. **condensation** [DSB23]. **condensed** [LWF<sup>+</sup>22]. **condition**  
 [GM22, MT20b, YAO20]. **conditions** [CX21b, FM21, LGJF22, PSMPB21].  
**conditions-mechanistic** [LGJF22]. **conductance** [KTM<sup>+</sup>23]. **conducting**  
 [LDT<sup>+</sup>22]. **conductivity** [KTM<sup>+</sup>23, RTB23]. **configuration**  
 [CV22, MR21, MPR22, PHS<sup>+</sup>20, SBD<sup>+</sup>21, WMZJ20].  
**configuration-interaction** [WMZJ20]. **configuration-space** [SBD<sup>+</sup>21].  
**configurational** [BAO<sup>+</sup>20]. **confined** [JC20]. **confinements** [AK20].  
**Confining** [VCRP23]. **Conformation** [KK23, DF22]. **Conformational**  
 [DA22, MVV22, OM22, TPZ<sup>+</sup>20, FBP<sup>+</sup>22, KN21, OC23, PDC23, SS20,  
 STR20, TTH<sup>+</sup>21a, TZS<sup>+</sup>22, WSV20, ZGZC20]. **Conformations**  
 [XZX<sup>+</sup>22, KGS<sup>+</sup>22]. **conformer** [JGK<sup>+</sup>22, JGK<sup>+</sup>22]. **Conformer-RL**  
 [JGK<sup>+</sup>22]. **Conformers** [ONC20]. **congeners** [POPGS22]. **conical** [AIV20].  
**conjugated** [CBF<sup>+</sup>20, FCB23, KZJ22]. **connection** [MPV22]. **Conquer**  
 [JGM21, FKT21, NN20, SY21]. **consequences** [SBD<sup>+</sup>21]. **conservation**  
 [CH23]. **considering** [SAZ<sup>+</sup>23]. **consistent** [CV22, CQSG20, CTPJH22,  
 LB21, LB22, NSH23, PW20, SLB23, SKKK20, VWJ23]. **Constant**  
 [SDH23, FNY21, SSS<sup>+</sup>20a]. **constants**  
 [LGM20, LGM22, SYS<sup>+</sup>21, dCVARN20]. **constrained**  
 [FNY21, MWK<sup>+</sup>20, TV22]. **constraints** [BMT<sup>+</sup>21, OAC23, PDL<sup>+</sup>21].  
**construction** [HC21, HD21, WMZJ20, ZFRM20]. **Contact** [CLS<sup>+</sup>20].  
**Contacts** [MKSS20]. **containing**  
 [CTBB20, DART21, NST<sup>+</sup>20, DMTR22, YLZ<sup>+</sup>22, ZGZ<sup>+</sup>20]. **context** [SS23].  
**continuous** [MSS20]. **Continuum**  
 [BBK20, ALA20, PCI23, STR20, UB20, VL22]. **contracted** [SM20].  
**contributing** [CH23]. **contribution** [AK20, Sán20]. **contributions**  
 [VWJ23]. **control** [DYGGM21]. **controlled** [CGMRVBAI22, FR21]. **controls**  
 [dARW<sup>+</sup>23]. **conventional** [SGGG22]. **convergence** [MT20b]. **conversion**

[FP23]. **converting** [VAP<sup>+</sup>21]. **cooperativity** [AK20, SJZ<sup>+</sup>21]. **Coordinate** [AD20, BCN22, dSCCN21, PBM21]. **coordinates** [ABTM22, BLB20, LL21b, WHJM23]. **coordinating** [Brz23]. **Coordination** [MVP<sup>+</sup>20, YMSS23, CVGVN<sup>+</sup>20, SK23, TLS23]. **copolymer** [LEP<sup>+</sup>21]. **copolymer/ionic** [LEP<sup>+</sup>21]. **copolymers** [BSR22]. **copper** [RLHG<sup>+</sup>23]. **Core** [NRH<sup>+</sup>20, MCP23, PDGD23, Pil20, SAZ<sup>+</sup>23]. **Core-Substituted** [NRH<sup>+</sup>20]. **corrected** [AS21, CHVF21, CTBB20, GAP21, HCS<sup>+</sup>20, KDLP21, LB21, LB22, SLB23]. **Correcting** [ÓLP<sup>+</sup>20]. **correction** [ASW20, BJ22, DYGM21, NI22, VL22]. **correction-scaling** [ASW20]. **Corrections** [HFPS20, POPGS22]. **correlated** [SM22a]. **Correlation** [NSH23, AA20, HM21, MH22, MPR22, NTK21, PW20, RMJ21, Sán20, SPSH20, SSO<sup>+</sup>20, TV22]. **correlations** [AS20, YW20]. **corresponding** [HSG21]. **corrole** [ASL<sup>+</sup>20]. **COSMO** [GSH23, SHHH22, VAL20]. **COSMO-RS** [SHHH22, VAL20]. **cosolvent** [TTH<sup>+</sup>21a]. **cost** [CK22, DKB23]. **costly** [CSWW20]. **Coulomb** [CQSG20]. **coumarin** [ZRSST20]. **coumarin-schiff** [ZRSST20]. **Counterion** [SLR<sup>+</sup>20]. **counterparts** [NG20]. **counterpoise** [NI22]. **Coupled** [BWM20, BS23, BTSB22, BSF20, DC22b, FB21, GRBN21, HPM<sup>+</sup>21, RCC<sup>+</sup>20, RDB23, WGKG20, XCJ20]. **coupled-cluster** [BSF20, DC22b]. **coupling** [ABZ20b, AMM22, DZL<sup>+</sup>20, FCPG20, HCY<sup>+</sup>22, IMT<sup>+</sup>21, MML<sup>+</sup>23, POPGS22, Tou21, Wan23]. **couplings** [SBD<sup>+</sup>21, SCKH21]. **COV** [ONA<sup>+</sup>20, EIT<sup>+</sup>21, KLZ<sup>+</sup>23, PDC23, PPP21, PPRS22, SLMA21, YC23, UAC<sup>+</sup>23]. **CoV-2** [UAC<sup>+</sup>23]. **covalency** [ZBH<sup>+</sup>23]. **Covalent** [AWID<sup>+</sup>20, GSJ<sup>+</sup>23]. **Cover** [ABZ20a, Ano20a, Ano20b, Ano20p, Ano20t, Ano20u, Ano20v, Ano20w, Ano20x, Ano20y, Ano20z, Ano20-27, Ano20-28, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20l, Ano20m, Ano20n, Ano20o, Ano20q, Ano20r, Ano20s, BUNO22a, BBC<sup>+</sup>21b, BOPJ<sup>+</sup>21b, CX21a, ETT21a, GPM21a, GKA<sup>+</sup>23a, HAC<sup>+</sup>23a, KE23a, KFTB20a, KSS21a, KK22b, MLG<sup>+</sup>21a, QLW<sup>+</sup>22a, RPD<sup>+</sup>20b, SWM<sup>+</sup>20a, dRHB21, SSFS22a, TTH<sup>+</sup>21b, TCS<sup>+</sup>21b, VV20a, WLSC23b]. **COVID** [SLMA21]. **COVID-19** [SLMA21]. **Cp** [HSG21, WLZM20]. **CR** [WLZM20, Wan23]. **create** [ZK23]. **created** [ARR22a]. **creating** [LKM20]. **Criegee** [SK20]. **Critical** [SB20, dSCCN21, MT20b]. **cross** [ABZ20b, ALA20, CV22, KGTL21, ZK23, dBCdL20]. **cross-coupling** [ABZ20b]. **cross-link-assisted** [KGTL21]. **cross-platform** [ZK23]. **cross-sections** [CV22, dBCdL20]. **crucial** [KE23b, MBBU23]. **cryo** [LSP23]. **cryo-EM** [LSP23]. **Crystal** [GLC<sup>+</sup>22, AK20, CX23, KZP22, MZ21, RDS<sup>+</sup>20]. **crystallin** [FLT23]. **Crystalline** [HZG<sup>+</sup>20, Cer22, PDGD22]. **crystals** [LT23, LWF<sup>+</sup>22, NMFI21]. **Cs** [SL20]. **CSiGaAl** [DC22a]. **CsPbBr** [BBL<sup>+</sup>22]. **Cu** [MH20, AD20, JGSA22, LZW<sup>+</sup>23, PP23, SPSH20]. **cube** [Bal20b]. **cupric** [XZZ<sup>+</sup>20]. **Current** [BSL20, SPT21, SZL23]. **Current-Flow** [BSL20]. **Curvature** [MA23a]. **Curvature-weighted** [MA23a]. **cut** [WKL22]. **cut-offs** [WKL22]. **cutoff** [DO20].

**cyanomethylation** [DSK21]. **cycle** [Dor20, MKB<sup>+</sup>21]. **cyclin** [TWT<sup>+</sup>22]. **cyclin-dependent** [TWT<sup>+</sup>22]. **cyclization** [TYZ20]. **cycloaddition** [KZJ22, MGCM21, NMMC21, SVTK<sup>+</sup>22, SMB<sup>+</sup>23]. **cyclobutanes** [HCY<sup>+</sup>22]. **cyclocondensation** [MIP<sup>+</sup>22]. **cyclooctatetraene** [KK22c]. **cyclopenta** [MSE<sup>+</sup>21]. **cyclopropane** [WG20]. **cyclotrimerization** [ZMH<sup>+</sup>21]. **cysteine** [dSCCN21]. **cytosine** [LRqG<sup>+</sup>22].

**D** [BBY<sup>+</sup>21, DF22, FLT23, GSJ<sup>+</sup>23, Pan23, PSM<sup>+</sup>20, SS20, TPZ<sup>+</sup>20, TZS<sup>+</sup>22, WKL22, dCVARN20]. **D-crystallin** [FLT23]. **D3** [FBM<sup>+</sup>23, RMJ21]. **D4** [NG20]. **D614G** [ONA<sup>+</sup>20]. **damaged** [CGMRVBAl22, LRqG<sup>+</sup>22]. **Data** [BK22, SK20, TV22, XZ20, BMT<sup>+</sup>21, GG22, IMT<sup>+</sup>21, LL22, SWLC22]. **Data-driven** [TV22]. **database** [AZKM22, CBB<sup>+</sup>21, LRKD23, GLC<sup>+</sup>22]. **databases** [LGD<sup>+</sup>20, ZK23]. **datasets** [KZOV23]. **Dative** [PTP23]. **DD** [CD20]. **DD-peptidase** [CD20]. **deacylation** [CD20]. **deal** [DWSX20]. **Deciphering** [HD21]. **decker** [AS23]. **Decoding** [MIP<sup>+</sup>22]. **decomposed** [NVBG23]. **decomposition** [AV20, AK20, CL23, HUO23, JCMHT22, LHG<sup>+</sup>23, MGCM21, MT20b, SSM21, TSZ<sup>+</sup>21, ZG21]. **decomposition-based** [MT20b]. **decorporation** [SDK20]. **decreasing** [HD21]. **dedicated** [CBB<sup>+</sup>21]. **Deep** [LPP20, PMT<sup>+</sup>22, JGK<sup>+</sup>22, MLP22, WLSC23a]. **deeper** [DGM22]. **deeply** [PDGD23]. **DEER** [QLC<sup>+</sup>20]. **defective** [PSM<sup>+</sup>20, SPT21]. **defects** [CTBB20, GPEK<sup>+</sup>20, PGP<sup>+</sup>21, PKT21]. **Deformation** [FMFG20, NVBG23, RA20]. **degenerate** [NSKN21]. **degrees** [DB23]. **dehydration** [KSS21b, KSRB<sup>+</sup>21]. **dehydrogenated** [ONC20]. **delayed** [LYX<sup>+</sup>22]. **delivers** [ZWY<sup>+</sup>22]. **delivery** [AAID22]. **delocalization** [LKAT22, RTB23]. **delocalized** [BdLC21]. **Densities** [WG21, Pil20, SZL23, TAC<sup>+</sup>23, Wan21a, Wan21b]. **Density** [BBK20, CFOMCB<sup>+</sup>22, CWZD20, CMD<sup>+</sup>22, FMFG20, KZJ22, MLB<sup>+</sup>23, RMJ21, RA20, SK20, TANC23, YXGZ20, APS20, AS21, ABAQ<sup>+</sup>23, BWS20, BA22, Ben22, BSF20, BBK<sup>+</sup>21, BOPJ<sup>+</sup>21a, CHVF21, CPG21, Cer22, CQSG20, ĆPP<sup>+</sup>22, CTBB20, DZL<sup>+</sup>20, DOT22, EPT21, FB20, GH22a, GD23, GAP21, HM21, HCS<sup>+</sup>20, IYI<sup>+</sup>20, KZJ21, KS21, KdILC22, LRF<sup>+</sup>21, MWK<sup>+</sup>20, MNH21, MH22, MKK<sup>+</sup>22, MAM21, MFS22, MKB<sup>+</sup>21, MGCM21, MH20, MSE<sup>+</sup>21, MBBU23, MSS20, NG20, NSH23, NEG<sup>+</sup>20, NVBG23, NN20, OE20, OMC<sup>+</sup>20, RCC<sup>+</sup>20, RC22, RTB23, SDK20, SWF<sup>+</sup>20, dASRHB21, SC22, SMB<sup>+</sup>23, SSYB<sup>+</sup>20, SZP<sup>+</sup>20, TLS23, TT20, VV20b, WKCP21, XSP<sup>+</sup>23, ZHHS21, ZZ23a, dBcDL20]. **density-fitted** [BSF20]. **Density-functional** [TANC23, BWS20, NEG<sup>+</sup>20]. **Depend** [BWM20]. **Dependence** [JK21, YXGZ20, MH20, SBD<sup>+</sup>21]. **dependencies** [BK22]. **Dependent** [YXGZ20, BA22, CPG21, FB20, FNY21, IYI<sup>+</sup>20, IN23a, JRS20, MFS22, MSS20, Ngo21, OMC<sup>+</sup>20, SZL23, TWT<sup>+</sup>22, TANC23, XZW<sup>+</sup>21, XAD20]. **deposited** [VTdlM20]. **deposition** [MSA22a]. **Derivation** [FMFG20].

**derivative** [CC22]. **Derivatives** [GRN20, BHR<sup>+</sup>21, CFOMCB<sup>+</sup>22, KK22c, SEBE21, SGGG22, DMTR22, TANC23]. **describe** [GAP21, IK21]. **described** [KKAK23]. **Describing** [HPM<sup>+</sup>21, MH22, RLHG<sup>+</sup>23]. **Description** [BLP20, HRT<sup>+</sup>20, XCJ20, ZLLL22]. **descriptors** [BHR<sup>+</sup>21, CMD<sup>+</sup>22, COK22, GJMPVR<sup>+</sup>20, HBT<sup>+</sup>20, LGM20, LGM22, NTK21, TCS<sup>+</sup>21a, YGG<sup>+</sup>23]. **Design** [IW23, PAS<sup>+</sup>20, SEBE21, BBB<sup>+</sup>23, DSK21, GLC<sup>+</sup>22, HKFT21, LSP23, LYX<sup>+</sup>22, LHH<sup>+</sup>23, NPGP23, PMT<sup>+</sup>22, PSB<sup>+</sup>22, RKC21, RDK<sup>+</sup>22, SHP<sup>+</sup>23, YYZ<sup>+</sup>21, ZZG<sup>+</sup>21, ZBH<sup>+</sup>23]. **designs** [YBS<sup>+</sup>20]. **desirable** [NPGP23]. **detailed** [NP23, SY21]. **details** [TYZ20]. **determinant** [BTSB22]. **Determination** [NNT<sup>+</sup>20, CST23, FKT21]. **determines** [HYA<sup>+</sup>20]. **Determining** [WZZ<sup>+</sup>20, KPHV23]. **deterministic** [TS21]. **Developing** [HKFT21]. **Development** [KG23, LRqG<sup>+</sup>22, SKL23, SHH<sup>+</sup>23b, SHH<sup>+</sup>23a, WSL<sup>+</sup>20, GKO<sup>+</sup>22]. **developments** [VWFR21]. **devices** [AMF<sup>+</sup>20, LAM<sup>+</sup>23, SPT21]. **DFT** [TANC23, AK20, AS23, ABNG22, BSR22, CS20, CL23, DK23, DSK21, FCB23, FBM<sup>+</sup>23, FV20, HS22, JMV21, KKAK23, LCC<sup>+</sup>21, LT23, LDT<sup>+</sup>22, MPOC21, MJS<sup>+</sup>23, MCD22, MK22b, NG20, RLHG<sup>+</sup>23, SVDS21, SB20, TANC23, TMO<sup>+</sup>21, WD20, WS21, WKG<sup>+</sup>23, YC23, ZRSST20, ZDBZ20]. **DFT-D4** [NG20]. **DFT/MRCI** [ZRSST20]. **Di-** [KZP22]. **diagnostic** [SD21]. **diagonalization** [BMT23, MB21, WFLZ23]. **diagonalization-free** [MB21]. **diagrammatic** [HD21]. **diagrams** [PDC23, VFCG20]. **dianionic** [DPSG20]. **diaqua** [MVP<sup>+</sup>20]. **diatomic** [AA20, Tze21]. **diatomics** [KW22]. **diazadiboretidine** [NHFS21]. **dicarboranyl** [PGP<sup>+</sup>23]. **dications** [SMH21]. **dichalcogenide** [PSM<sup>+</sup>20]. **dichroism** [MSA22b]. **dichromium** [MVP<sup>+</sup>20]. **dicopper** [MVP<sup>+</sup>20]. **dielectric** [RMS<sup>+</sup>23]. **Diels** [MNZGO<sup>+</sup>20, MGCM21, NMCM21, SSYB<sup>+</sup>20]. **diene** [NMCM21]. **differences** [WFB22]. **different** [DO20, DWSX20, KK23, Sts20, WS21]. **differential** [SD21]. **diffuse** [MCP23]. **diffusion** [BUNO22b, CGMRVBAl22, FNY21, PFSC20, RGGD21, SM22b, UKBD23]. **diffusion-controlled** [CGMRVBAl22]. **diffusivity** [NS22]. **difluoro** [SKGG23]. **difluorocarbene** [ZS22]. **digestion** [Nee23]. **dihalogens** [RZS<sup>+</sup>23]. **dihedral** [RR22]. **Diimides** [NRH<sup>+</sup>20]. **diimine** [WCD<sup>+</sup>23]. **diketones** [AV20]. **dimensional** [GVJ<sup>+</sup>22, KGS<sup>+</sup>21, LWLC21, PPV<sup>+</sup>21, STB<sup>+</sup>20, YAO20]. **dimer** [BCN22, JC20, Kop22a, SAZ<sup>+</sup>23, YrYqLhC23]. **Dimerization** [WGKG20, BVC<sup>+</sup>23]. **dimers** [BD22, MC23, WCD<sup>+</sup>23]. **dinickel** [LLKS23]. **dinitrate** [GJL21]. **dinitrogen** [DGM22, KJV23, SK23]. **dioxaphosphole** [MSE<sup>+</sup>21]. **dioxaphosphole-2-sulfide** [MSE<sup>+</sup>21]. **Dioxide** [SB20, ZSD<sup>+</sup>20]. **Dipolar** [SVTK<sup>+</sup>22]. **dipole** [BS23, BSF20, HPG20, LRKD23]. **dipole-coupled** [BS23]. **Direct** [FMFG20, YW20]. **Directing** [AD20]. **directions** [BBSFA22, MAM21, YAO20]. **discovery** [CDCT21, LHH<sup>+</sup>23, MNBG<sup>+</sup>21]. **Discriminating** [CX23]. **Disentanglement** [CB20]. **Dismantlement** [YOCMA23]. **disorder** [DB23]. **disordered** [SY21]. **disparity** [DWSX20]. **dispersion**

[CTBB20, MBBU23, RMJ21]. **dispersion-corrected** [CTBB20]. **displacement** [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]. **Distributed** [GJMPVR+20, LRKD23]. **distribution** [IN23b, QLC+20, Tou21]. **distributions** [LBH+22, MVV22, SKKK20]. **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** [FVSS20, FBP+22, HKS20, SBFSJMLU23, SGGG22]. **DNN** [XLW+22]. **do** [CPG21, GUCCR20, ZGZC20]. **Dock** [Min20, AG21, PSB+22]. **Docking** [XZ20, BAO+20, CFOMCB+22, LYKS23, MZMK+21, MSA22a, PPP21, RKC21, TZS+22, VWP+22, YC23]. **dodecahedrane** [JC20]. **dodecyl** [ZK21]. **DOI** [MT20a]. **Domain** [PT20, PW20, TLD+22, BVC+23, GRBN21, San21]. **Domain-based** [PW20]. **donation** [GAG20]. **donor** [DDSM23, PTP23]. **dopamine** [TPZ+20, TZS+22]. **doped** [DZL+20, DOT22, WMJ+22, ZDBZ20]. **Double** [FV20, OMC+20, AQMM+23, BOPJ+21a, CPG21]. **double-hybrid** [BOPJ+21a]. **Doubles** [HFPS20]. **downregulation** [CSP20]. **downward** [ETT21b]. **DPC** [ZK21]. **drive** [RLR+20]. **driven** [AIV20, SBFSJMLU23, San21, SSS+20b, TV22, YJZ+22]. **Drude** [BS23, KLP+22, KYM20, LJ20, ODL20]. **Drug** [SLMA21, AAID22, DYGM21, HKFT21, LSP23, RKC21, RDK+22]. **drug-delivery** [AAID22]. **drug-like** [DYGM21]. **druglike** [SHH+23b]. **drugs** [HS22, HS23, HBM+20, NST+20, PRH20, dCRM21]. **Dual** [YW20, MPP23]. **dual-atom** [DLH+23]. **Dual-hybrid** [YW20]. **due** [FBP+22, MAM21, ÖLP+20]. **dyes** [TMO+21]. **dynamic** [BAO+20, MPOC21, MK22a, SYS+21]. **dynamical** [RR22, SZL23]. **dynamically** [MT20b, TWT+22]. **Dynamics** [FMFG20, HHL+20, KUNT20, YXGZ20, Zac20, AiS+21, ALA+22, BUNO22b, BAO+20, BBL+22, CDCT21, CSP20, CST23, DHN+21, FNY21, FBP+22, GGK20, GG22, JRS20, JKK+21, KR23, KOD21, KLP+22, LL21a, LKM20, LHH+21, LEP+21, MN20, MKK+22, MGB+22, MSA22a, MAP+20, NLC23, 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, SSFS22b, SKKK20, SCCZ21, TPB22, UKBD23, VCRP23, WSV20, WCT+23, WFBB22, WKD+21, YC23, ZG21, ZWY+22, ZFRM20].

**E-fields** [AMF+20]. **E4** [WS21]. **ebselen** [YC23]. **EDA**

[DGM22, GM22, GKA<sup>+23b</sup>]. **EDA-NOCV** [DGM22, GM22, GKA<sup>+23b</sup>]. **edge** [CS23]. **Effect** [AD20, DLH<sup>+23</sup>, GRN20, JC20, ARR22a, CBF<sup>+20</sup>, DO20, FVSS20, JMK<sup>+20</sup>, KPHV23, KEK23, LK22, LLZ<sup>+23</sup>, MAM21, MEKH22, PRH20, Sts20, SCZ<sup>+21</sup>, XZW<sup>+21</sup>]. **effective** [BBC<sup>+21a</sup>, KKAK23, UB20]. **Effects** [DK23, JFZ<sup>+20</sup>, KPDB22, KTM<sup>+23</sup>, MSA22a, SLR<sup>+20</sup>, SGT<sup>+20</sup>, CX21b, FBP<sup>+22</sup>, GCP22, GAG20, KWYN23, MCD22, PCI23, SSSA23, dCVARN20]. **efficiency** [FYIO23]. **Efficient** [CSGVF<sup>+20</sup>, LMPT21, MN20, MR21, MKB<sup>+21</sup>, MT20b, PPV<sup>+21</sup>, RCC21, XLW<sup>+22</sup>, AD23, DYGM21, EK20a, KG23, KSRKS21, ZZG<sup>+21</sup>]. **effort** [POvG21]. **eigenvalues** [KDLP21]. **Eighth** [PSMPB21]. **Eighth-Shell** [PSMPB21]. **elacestrant** [CSP20]. **elastic** [KOD21, MA23a, MA23b, MMAZ<sup>+23</sup>, ZLLL22]. **Electric** [PL22, SHM<sup>+20</sup>, ZG21]. **electride** [DSC20]. **electrocatalysts** [AR20]. **electrochemical** [KDLP21]. **Electrocyclization** [PC21]. **electrode** [DOT22]. **electrolyte** [LEP<sup>+21</sup>]. **electrolytes** [EG20, HM21]. **Electron** [KZJ22, BJ22, BBC<sup>+21a</sup>, EVKL21, EPT21, IN23a, KZJ21, LKT21, LKAT22, LT23, MH22, MAM21, PTP23, RCC<sup>+20</sup>, RNP20, RTB23, SS20, SPSH20, SMB<sup>+23</sup>, SSO<sup>+20</sup>, SZL23, TAC<sup>+23</sup>, dBCdL20]. **electronegativity** [Vyb23]. **Electronic** [DGSB<sup>+20</sup>, SBFSJMLU23, SM22b, SCKH21, TT20, ABAQ<sup>+23</sup>, AMF<sup>+20</sup>, BTSB22, CC22, HSG21, IK21, JMV21, KWYN23, KPDB22, Kop22a, LXP<sup>+22</sup>, LAM<sup>+23</sup>, MNH21, MML<sup>+23</sup>, MNZGO<sup>+20</sup>, MSA22b, MP23, NHFS21, OSHT20, PSM<sup>+20</sup>, RvWH23, RCC<sup>+20</sup>, SGT<sup>+20</sup>, STB<sup>+20</sup>, TPZ<sup>+20</sup>, TSH<sup>+23</sup>, VM23, WMJ<sup>+22</sup>, XZW<sup>+21</sup>]. **electrons** [MP23, PDGD23]. **electrooxidation** [DOT22]. **electrophilicities** [HBT<sup>+20</sup>]. **Electrophilicity** [PC23]. **electrostatic** [AS20, HS23, JGGPN21, LWLC21, LDT<sup>+22</sup>, MMK<sup>+20</sup>, ÖLP<sup>+20</sup>, UB20, VL22, ZZ23a]. **Electrostatically** [TSR21]. **Electrostatics** [HRT<sup>+20</sup>, SCvW22, YFH<sup>+21</sup>]. **element** [PLZT23]. **elementary** [DGSB<sup>+20</sup>, SYS<sup>+21</sup>]. **Elementometalation** [WLZM20]. **elements** [GPM21b, Klo22, NUK21, RCC21, RNP20]. **elimination** [KZJ21]. **Elongation** [MMK<sup>+20</sup>]. **Elucidating** [NST<sup>+20</sup>]. **Elucidation** [SKGG23, HRTSS<sup>+20</sup>]. **elusive** [DDSM23]. **embedded** [TSR21]. **embedding** [DGSB<sup>+20</sup>, IRB<sup>+23</sup>, LWLC21, LDT<sup>+22</sup>, MMK<sup>+20</sup>, UB20]. **embrittlement** [ZFRM20]. **emission** [AS20, FB20]. **emitters** [LYX<sup>+22</sup>]. **Empirical** [LJ20, KB22, PWX<sup>+20</sup>, PNT<sup>+22</sup>, RLHG<sup>+23</sup>]. **employing** [MAI22]. **enabled** [BCN22, LBH<sup>+22</sup>]. **Encapsulation** [CBF<sup>+20</sup>, DSC20, SSSA23]. **Encoding** [GJMPB<sup>+20</sup>]. **End** [MXM20, SK23, TANC23, TTK23]. **end-group** [TANC23]. **end-on** [SK23]. **End-Point** [MXM20, TTK23]. **ended** [GSD<sup>+22</sup>]. **Endo** [Jab22a]. **Endo-** [Jab22a]. **endohedral** [DA22, LXP<sup>+22</sup>]. **endpoint** [SHH<sup>+23b</sup>, SHH<sup>+23a</sup>]. **ene** [SMB<sup>+23</sup>]. **energetic** [JMV21]. **energetically** [NSKN21]. **Energetics** [HHL<sup>+20</sup>, NG20, PM21, WGKG20]. **Energies** [BBK20, FMFG20, HFPS20, MFC20, NRH<sup>+20</sup>, AD23, BBY<sup>+21</sup>, BOPJ<sup>+21a</sup>, BCN22, FCB23, Fed22, GZFSM21, HCS<sup>+20</sup>, KPHV23, LCC<sup>+21</sup>, MPP23,

MLB<sup>+</sup>23, MEKH22, MCP23, NTK21, ÖLP<sup>+</sup>20, OM22, PRF20, PFSC20, TTK23, TTT<sup>+</sup>21, VV21]. **Energy** [FKT21, GRN20, KPR23, LPP20, MXM20, Min20, NNT<sup>+</sup>20, SZLD20, YYS20, AV20, ARR22a, AK20, AA20, BBC20, BJ22, BBC<sup>+</sup>21a, BF22, CC22, CSGVF<sup>+</sup>20, CdSB<sup>+</sup>21, CSWW20, CSP20, DC22a, GH22a, GBM20, GVJ<sup>+</sup>22, HB21, HBM<sup>+</sup>20, HPM<sup>+</sup>21, JK21, JCMHT22, JGM21, KG23, KK23, KFTB20b, Kop22b, Kos22, LPF<sup>+</sup>23, LWF<sup>+</sup>22, LML<sup>+</sup>23, LHG<sup>+</sup>23, MML<sup>+</sup>23, MN20, MSL<sup>+</sup>20, MGCM21, MBBU23, NUK21, NTK21, NMFI21, NI22, NML21, OKI<sup>+</sup>21, PPV<sup>+</sup>21, PDC23, RDB23, RH21, Sán20, SSS<sup>+</sup>20a, SY21, SDH23, Sts20, SCCZ21, SHH<sup>+</sup>23b, SHH<sup>+</sup>23a, TWT<sup>+</sup>22, TSZ<sup>+</sup>21, TM20, TSH<sup>+</sup>23, VL22, Vyb23, WCT<sup>+</sup>23, WFBB22, XLW<sup>+</sup>22, YBS<sup>+</sup>20, YFH<sup>+</sup>21, ZK21]. **energy-adjusted** [GH22a]. **Energy-based** [FKT21, LWF<sup>+</sup>22]. **energy-related** [CdSB<sup>+</sup>21]. **enforced** [WCD<sup>+</sup>23]. **engineering** [SZP<sup>+</sup>20]. **enhance** [YYZ<sup>+</sup>21]. **Enhanced** [FMFG20, OC23, WLSC23a, DWSX20, KLZ<sup>+</sup>23, LGC21, MH20, MMAZ<sup>+</sup>23, ONA<sup>+</sup>20]. **enol** [LKAT22]. **enrichments** [KDP<sup>+</sup>22]. **ensemble** [HTFY21, HBM<sup>+</sup>20, QLC<sup>+</sup>20, RD23, XLW<sup>+</sup>22]. **ensembles** [NML21]. **entangled** [WKD<sup>+</sup>21]. **entatic** [RLHG<sup>+</sup>23]. **enter** [APS20]. **enthalpies** [Dor20]. **entirely** [BdLC21]. **entropy** [YJZ<sup>+</sup>22]. **entropy-driven** [YJZ<sup>+</sup>22]. **entry** [GG22]. **ENUF** [YLZ<sup>+</sup>20]. **Enumeration** [SZLD20]. **environment** [BBB<sup>+</sup>23, KCF<sup>+</sup>20, NUK21]. **enynes** [HCY<sup>+</sup>22]. **Enzymatic** [SHM<sup>+</sup>20, PRF20]. **enzyme** [DPSG20]. **ePharmer** [MLG<sup>+</sup>21b]. **epidermal** [BHR<sup>+</sup>21]. **EPISOL** [CKH23]. **epoxides** [WKG<sup>+</sup>23]. **equalization** [Vyb23]. **equation** [NSRK21, RCC21, SCvW22]. **equations** [MB21, MT20b]. **equatorial** [SVDS21]. **equilibria** [CM20a, CA22]. **Equilibrium** [dSCCN21, KS21]. **Erratum** [MT20a]. **error** [KM22, UKBD23]. **ESCASA** [LL21b]. **essential** [GLC<sup>+</sup>22]. **establish** [RCC<sup>+</sup>20]. **estimate** [LRKD23]. **estimates** [AD23]. **Estimating** [LBH<sup>+</sup>22, Ngo21, BK22]. **estimation** [JGM21, KZP22, KG23, LL21b, TTK23]. **Estimations** [TTT<sup>+</sup>21]. **estimator** [AZKM22, Vyb23]. **estrogen** [CSP20]. **ethanol** [KGS<sup>+</sup>22]. **ethyl** [MIP<sup>+</sup>22]. **ethylene** [HCY<sup>+</sup>22, MCD22, PLZT23, SVTK<sup>+</sup>22, SJZ<sup>+</sup>21]. **ethylenediamine** [MIP<sup>+</sup>22]. **ETS** [SBB<sup>+</sup>22]. **ETS-NOCV-based** [SBB<sup>+</sup>22]. **Eu** [ALA<sup>+</sup>22]. **europium** [HRTSS<sup>+</sup>20]. **Evaluating** [TZS<sup>+</sup>22]. **Evaluation** [BHR<sup>+</sup>21, KS21, MZMK<sup>+</sup>21, MCD22, PRH20, VAL20, BBB<sup>+</sup>23, DWZ22, Gao20, LLZ<sup>+</sup>23, MLB<sup>+</sup>23, SEBE21, SSS<sup>+</sup>20a, ZZ23a, SHH<sup>+</sup>23a]. **events** [RLR<sup>+</sup>20, RD23, WRBT21]. **Evolution** [GJL21, MM20, CG20, DLH<sup>+</sup>23, KdILC22, MIP<sup>+</sup>22, PSB<sup>+</sup>22, WMJ<sup>+</sup>22, YYS20]. **Evolutionary** [CH23]. **Ewald** [Pan23, YLZ<sup>+</sup>20]. **Examining** [NGD22]. **Exchange** [BBK20, MBBU23, AA20, HM21, JKS23, KN21, KK23, KKAK23, LKT21, MH22, MGB<sup>+</sup>22, MZMK<sup>+</sup>21, RMJ21, RR22, SEZ20, TV22, VV20b, XZX<sup>+</sup>22, YW20]. **exchange-correlation** [AA20, HM21, MH22]. **excision** [LRqG<sup>+</sup>22]. **Excitation** [HFPS20, HCS<sup>+</sup>20, NRH<sup>+</sup>20, FCB23, Kos22]. **excitations** [BOPJ<sup>+</sup>21a]. **Excited** [AIV20, Tou21, VM23, BMT23, CG20, CPG21, FCB23, FB21, Gie21, HD21, HPM<sup>+</sup>21, IK21, JCMHT22, KL20, LHH<sup>+</sup>21,

OSHT20, OMC<sup>+</sup>20, RDS<sup>+</sup>20, Sts20, WD20, WFLZ23, ZRSST20].  
**Excited-state** [AIV20, WD20, ZRSST20]. **excitonic** [SBD<sup>+</sup>21]. **Exhaustive** [BAO<sup>+</sup>20, SZLD20]. **exhibited** [Wan23]. **exhibiting** [LYX<sup>+</sup>22]. **existence** [OAC23]. **exohedral** [Jab22a]. **expanded** [CKH23, NML21]. **experimental** [AZKM22, BMT<sup>+</sup>21, GG22, HBT<sup>+</sup>20]. **Explicit** [MGB<sup>+</sup>22, CCHS23, LKT21, RPD<sup>+</sup>20a, WLSC23a]. **explicit-implicit** [RPD<sup>+</sup>20a]. **explicitly** [LRKD23, SM22a]. **Exploration** [GVJ<sup>+</sup>22, OOY20, RKC21, LGJF22, LLKS23, OC23, OKI<sup>+</sup>21, RSHG23, SDK20, San21].  
**Explorer** [SSFS22b]. **Exploring** [AVM21, MSL<sup>+</sup>20, NTK21, SCCZ21, YC23]. **expressed** [HCS<sup>+</sup>20].  
**expression** [UKBD23]. **Extended** [GX20, RGGD21, DWSX20, KGD<sup>+</sup>21, NBE<sup>+</sup>23, PSMPB21]. **Extension** [AYO20, JCMHT22]. **External** [GD23, BW22b]. **extrapolation** [SCKH21].  
**extremely** [JKK<sup>+</sup>21, RBM<sup>+</sup>23].

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

**fluorescence** [AS21, LYX<sup>+</sup>22]. **fluorescent** [ZRSST20]. **Fluorine** [OE20].  
**flux** [MNZGO<sup>+</sup>20]. **fly** [OSHT20, RBM<sup>+</sup>23]. **focal** [BSF20]. **focal-point**  
 [BSF20]. **Fock** [BTSB22, BBK20, NSH23, NI22]. **Fold** [CLS<sup>+</sup>20]. **Folding**  
 [GG22, CH23, SSS<sup>+</sup>20b]. **Following** [CG20, KdILC22, ETT21b]. **Force**  
 [BAC20, LJ20, QB20, WSL<sup>+</sup>20, ALA<sup>+</sup>22, BJ22, DHD21, FVSS20, GKO<sup>+</sup>22,  
 KLP<sup>+</sup>22, KYM20, LRqG<sup>+</sup>22, MT21, MNZGO<sup>+</sup>20, MAKZ23, ODL20,  
 PPV<sup>+</sup>21, PLP<sup>+</sup>20, TPB22, WLWR22, YFH<sup>+</sup>21, ZWY<sup>+</sup>22]. **force-field**  
 [GKO<sup>+</sup>22]. **forces** [BW22b, KSP21, LCC<sup>+</sup>21]. **Form** [CWZD20]. **formally**  
 [SSP23]. **formamide** [NHFS21]. **Formation**  
 [GOY20, LZW<sup>+</sup>23, HL20, KPDB22, MDO<sup>+</sup>20, SSS<sup>+</sup>20a, SKGG23, ZZ23b].  
**formats** [VAP<sup>+</sup>21]. **formic** [FP23]. **forms** [DSC20]. **formula** [Pan23].  
**formulas** [IN23a]. **formulation** [CK22]. **formulations** [SCvW22].  
**foundation** [TSH<sup>+</sup>23]. **four** [DSB23, KWYN23]. **four-component**  
 [KWYN23]. **four-membered** [DSB23]. **Fourier** [YLZ<sup>+</sup>20]. **Fractional**  
 [ASW20]. **fracture** [MMAZ<sup>+</sup>23]. **Fragment** [CLS<sup>+</sup>20, KUNT20, AKN<sup>+</sup>20,  
 BSS<sup>+</sup>22, BBC<sup>+</sup>21a, Fed22, NUK21, NAN<sup>+</sup>23, TWT<sup>+</sup>22, UB20, ZK23].  
**fragment-based** [UB20]. **Fragment-Free** [CLS<sup>+</sup>20]. **Fragmentation**  
 [AKN<sup>+</sup>20, SD21, LWF<sup>+</sup>22, VWJ23]. **FRAGMENTISE** [ZK23]. **Fragments**  
 [AD23, LML<sup>+</sup>23, PTP23, RTB23, SSP23]. **Fragments-in-fragments**  
 [AD23]. **Framework**  
 [GRN20, LPP20, CM20a, GUCCR20, HRTSS<sup>+</sup>20, KZJ21, WMZJ20, WFBB22].  
**frameworks** [WP20]. **Free** [BBC20, CLS<sup>+</sup>20, FMFG20, GBM20, JGM21,  
 KK23, MXM20, Min20, NNT<sup>+</sup>20, SZLD20, ZK21, AQMM<sup>+</sup>23, BF22, BCN22,  
 CSP20, GVJ<sup>+</sup>22, GH22b, HB21, HBM<sup>+</sup>20, LPF<sup>+</sup>23, MPP23, MN20, MB21,  
 NML21, ÖLP<sup>+</sup>20, PPV<sup>+</sup>21, PDC23, SY21, SCCZ21, SHH<sup>+</sup>23b, SHH<sup>+</sup>23a,  
 TM20, TTK23, TYZ20, WFBB22, YBS<sup>+</sup>20, YIO20]. **Free-energy**  
 [GBM20, KK23, SY21]. **frequencies** [OM23]. **frequency** [IN23a, SZL23].  
**frequency-dependent** [IN23a, SZL23]. **friendly** [SKS21, ZK23]. **fromage**  
 [RDS<sup>+</sup>20]. **Front** [HAC<sup>+</sup>23a, WLSC23b]. **frustrated** [FP22, ZS22].  
**FSATOOL** [SWLC22, WLSC23a, ZGZC20]. **Fukui** [GFRNC21, GUCCR20].  
**full** [RMJ21, YLZ<sup>+</sup>22]. **fullerene** [AK20, YLZ<sup>+</sup>22]. **fullerenes**  
 [SSSA23, WKCP21]. **Fulleride** [AS23]. **Fulleride-metal** [AS23]. **fully**  
 [LEP<sup>+</sup>21]. **fumarate** [CFOMCB<sup>+</sup>22]. **function** [AV20, BPL<sup>+</sup>22, ĆPP<sup>+</sup>22,  
 IN23b, KFTB20b, KPR23, KDP<sup>+</sup>22, SWF<sup>+</sup>20, Tou21, WMZJ20, YFH<sup>+</sup>21].  
**function-based** [AV20]. **function-related** [BPL<sup>+</sup>22]. **Functional**  
 [BBK20, CWZD20, SK20, YXGZ20, APS20, AS21, ABAQ<sup>+</sup>23, BWS20, BA22,  
 Ben22, CFOMCB<sup>+</sup>22, CHVF21, CPG21, Cer22, CMD<sup>+</sup>22, CTBB20, DZL<sup>+</sup>20,  
 DOT22, FB20, GH22a, GD23, HM21, HCS<sup>+</sup>20, IYI<sup>+</sup>20, KS21, KdILC22,  
 LRF<sup>+</sup>21, MWK<sup>+</sup>20, MNH21, MLB<sup>+</sup>23, MFS22, MKB<sup>+</sup>21, MGCM21, MH20,  
 MSE<sup>+</sup>21, MSS20, NEG<sup>+</sup>20, NN20, OE20, OMC<sup>+</sup>20, RC22, SDK20,  
 dASRHB21, SC22, SSYB<sup>+</sup>20, SZP<sup>+</sup>20, TANC23, TLS23, WKCP21, ZHHS21,  
 ZGZ<sup>+</sup>20]. **functionalization** [SBFSJMLU23]. **Functionalized**  
 [LR20, FP23, HCY<sup>+</sup>22, KGS<sup>+</sup>21, KJV23, YYZ<sup>+</sup>21]. **functionals**  
 [BOPJ<sup>+</sup>21a, DK23, GAP21, HM21, HCS<sup>+</sup>20, MH22, MN20, MKK<sup>+</sup>22, NG20,

RMJ21, TV22, WS21]. **Functions**

[GJMPB<sup>+</sup>20, CC22, CKH23, CV22, GUCCR20, IN23b, Kop22b, MAM<sup>+</sup>23, MEKH22, MFS22, MCP23, SM20, SCZ<sup>+</sup>21, TAC<sup>+</sup>23]. **fusion** [EIT<sup>+</sup>21]. **future** [IRB<sup>+</sup>23]. **Fuzzy** [GJMPB<sup>+</sup>20, GJMPVR<sup>+</sup>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<sup>+</sup>23]. **gamble** [GNL<sup>+</sup>22]. **Gas** [OM23, AZKM22, APR21,

DC22b, IMT<sup>+</sup>21, KGS<sup>+</sup>22, MSYS23, MK22b, SW21, WG20]. **Gas-phase**

[OM23, AZKM22, DC22b, IMT<sup>+</sup>21, SW21]. **gases** [YMSS23]. **Gaussian**

[AAL21, BP22, GRN20, GH22b, IN23b, LB21, LB22, SS23, SLB23].

**Gaussians** [ALA20]. **GDIS** [VWFR21]. **Ge**

[LXP<sup>+</sup>22, WMJ<sup>+</sup>22, Wan23, GPM21b, SGT<sup>+</sup>20]. **General**

[Gao20, RMJ21, UKBD23, VCL20]. **Generalized**

[GCL<sup>+</sup>20, HTFY21, SH23, VV20b, BMT<sup>+</sup>21, JKS23, LWF<sup>+</sup>22, NG20, XCJ20].

**Generalized-ensemble** [HTFY21]. **generate** [AG21]. **generated**

[WKG<sup>+</sup>23]. **Generating** [SHM<sup>+</sup>20, VAP<sup>+</sup>21]. **generation**

[AMF<sup>+</sup>20, DYGM21, EVKL21, Gao20, GSD<sup>+</sup>22, JGK<sup>+</sup>22, LYX<sup>+</sup>22, Nee23,

RB22, SM22a, TIK21]. **generative** [PMT<sup>+</sup>22]. **generic** [WFBB22]. **genetic**

[LHH<sup>+</sup>23, RDB23, SS20]. **genetic-algorithm** [LHH<sup>+</sup>23]. **Geometric**

[ETT21b, OAC23, DHD21]. **Geometrical**

[RLHG<sup>+</sup>23, GJMPVR<sup>+</sup>20, KTM<sup>+</sup>23]. **geometrically** [PFP<sup>+</sup>21].

**Geometries** [LXP<sup>+</sup>22, NG20, WD20]. **Geometry**

[LPP20, SBD<sup>+</sup>21, AZKM22, CMD<sup>+</sup>22, LLS22a, LL21b, MMK<sup>+</sup>20, OC23].

**germaboryne** [DDSM23]. **Ge**  $\equiv$  [DDSM23]. **GFN** [MKB<sup>+</sup>21, OM22].

**GFN-xTB** [MKB<sup>+</sup>21]. **GFP** [RPD<sup>+</sup>20a]. **giant** [WKCP21]. **GIAO**

[MPOC21]. **GIAO-NMR** [MPOC21]. **glassy** [Tou21]. **Glioblastoma**

[CM20b]. **Global** [CPG21, AZKM22, DC22a, MZ21, NAAP21, OC23,

OKI<sup>+</sup>21, RTB23, TTH<sup>+</sup>21a]. **glucose** [DOT22]. **Glycans** [KUNT20].

**glycine** [HB21, ONC20]. **glycoprotein** [ONA<sup>+</sup>20]. **glycoprotein-enhanced**

[ONA<sup>+</sup>20]. **glycosaminoglycan** [MGB<sup>+</sup>22]. **glycosaminoglycans**

[MZMK<sup>+</sup>21]. **goal** [NSRK21]. **goal-oriented** [NSRK21]. **GoGreenGo**

[PKT21]. **gold** [LL21a, NST<sup>+</sup>20, NSKN21, POPGS22]. **GPU** [ZKJ<sup>+</sup>23].

**GPU-specific** [ZKJ<sup>+</sup>23]. **gradient** [BMT<sup>+</sup>21, LC22, NG20, VV20b].

**gradients** [BSF20, VCL20]. **grafted** [GBM20]. **Grained** [MT20a, WSL<sup>+</sup>20,

WZZ<sup>+</sup>20, BS23, CST23, GWN21, KGTL21, LL21b, LL22, MT19, SSDL<sup>+</sup>23].

**grand** [GGK20, ZKJ<sup>+</sup>23]. **grand-canonical** [GGK20]. **graph**

[BCN22, CdSB<sup>+</sup>21, NGD22, RSHG23]. **graph-based** [RSHG23]. **Graphene**

[KK22c, BWS20, DZL<sup>+</sup>20, DOT22, RC22, SS23, SPT21, YC20, dCRM21].

**Graphene-induced** [KK22c]. **graphene-supported** [BWS20, DZL<sup>+</sup>20].

**Graphical** [SBG20, MLG<sup>+</sup>21b]. **Graphics** [GCL<sup>+</sup>20, DWZ22]. **Graphs**

[SBG20, DHD21, YGG<sup>+</sup>23]. **grasp** [BPDG21]. **greater** [LML<sup>+</sup>23]. **Gremlin**

[CM20b]. **Gremlin-1** [CM20b]. **Grid** [Min20, CP23]. **grid-based** [CP23].

**GROMACS** [LKM20, MPP23]. **Ground** [Kop22b, HPM<sup>+</sup>21, KBHG23, WD20]. **Ground-state** [Kop22b, KBHG23, WD20]. **Group** [LXP<sup>+</sup>22, SBG20, BPL<sup>+</sup>22, BD22, BBK<sup>+</sup>21, Brz22, DPSG20, GPM21b, KW22, Klo22, KBHG23, LGM22, NUK21, PB20, PT21, PLZT23, PP23, RMJ21, TANC23, TT20, WCD<sup>+</sup>23, XSP<sup>+</sup>23, ZS22, SMH21]. **Group-14** [LXP<sup>+</sup>22]. **group-CASPT2** [TT20]. **groups** [HPG20]. **growth** [BHR<sup>+</sup>21]. **GRP1** [PT20]. **guanidine** [RLHG<sup>+</sup>23]. **guanidine-quinoline** [RLHG<sup>+</sup>23]. **guanine** [XZX<sup>+</sup>22]. **guanosine** [XZX<sup>+</sup>22]. **guest** [BRNB21, GBM20, MJS<sup>+</sup>23, YLZ<sup>+</sup>22]. **guest-guest** [MJS<sup>+</sup>23]. **guests** [KPKS23]. **GUI** [KLP<sup>+</sup>22, QLC<sup>+</sup>20, SSMP23]. **Guide** [ARR22a, SSMP23]. **Guided** [CLS<sup>+</sup>20]. **Gulari** [VFCG20].

**H** [KPTT21, LR20, PGP<sup>+</sup>23, TTK23, WSV20, AWK<sup>+</sup>23, GAP21, GJL21, KPTT21, LML<sup>+</sup>23, LL21b, MCP23, MBBU23, OKI<sup>+</sup>21, YYS20, ZHHS21, dCVARN20]. **H-bonded** [LML<sup>+</sup>23]. **H/D** [dCVARN20]. **hairpin** [YFH<sup>+</sup>21, ZZ23b]. **halide** [APR21, dARW<sup>+</sup>23]. **halides** [AQMM<sup>+</sup>23]. **halogen** [CB20, JGGPN21, SJZ<sup>+</sup>21, ZBH<sup>+</sup>23]. **halogenated** [LK22]. **Hamiltonian** [IK21]. **Hamiltonians** [KKAK23]. **handling** [WHJM23]. **hardness** [GFRNC21]. **harmonic** [CS23, Cer22, EVKL21]. **Hartree** [BTSB22, BBK20, NSH23, NI22]. **having** [DC22a]. **HC** [BdLC21]. **HCl** [AWK<sup>+</sup>23]. **HCVpred** [MPuS<sup>+</sup>20]. **HD** [BBY<sup>+</sup>21]. **HDAC** [MIK<sup>+</sup>23]. **HDAC2** [MIK<sup>+</sup>23]. **HDAC2-selectivity** [MIK<sup>+</sup>23]. **H...** [ARR22b]. **heat** [BAO<sup>+</sup>20, SSYB<sup>+</sup>20]. **heat-shock** [BAO<sup>+</sup>20]. **heavy** [DART21, Klo22]. **Hedgehog** [Ban20]. **Heisenberg** [KKAK23]. **helical** [MVV22, SSS<sup>+</sup>20b]. **helices** [VCL20]. **helium** [BGS<sup>+</sup>20]. **Helix** [MKSS20, HTFY21, NYM22]. **helix-mimetic** [HTFY21]. **heme** [LYKS23, SWF<sup>+</sup>20, SWM<sup>+</sup>20b, LYKS23]. **hemodialysis** [MSA22a]. **hepatitis** [MPuS<sup>+</sup>20]. **heptagons** [IW23]. **Herzberg** [Tou21]. **hetero** [GPM21b]. **hetero-bileptic** [GPM21b]. **heterobimetallic** [ZMH<sup>+</sup>21]. **heterocycles** [BSS<sup>+</sup>22]. **heterocyclic** [FP22, JGSA22]. **heterointerface** [SZP<sup>+</sup>20]. **heterojunction** [TANC23]. **Heterolytic** [LR20]. **heteronuclear** [KW22, SJZ<sup>+</sup>21]. **heterostructures** [PSM<sup>+</sup>20]. **hexa** [FDK22]. **hexa-** [FDK22]. **hexane** [NS22]. **Hf** [DBE20, AWK<sup>+</sup>23]. **Hg** [SSS<sup>+</sup>20a]. **hidden** [GM22, SSP23]. **Hierarchical** [NN20, dASRHB21, AAFJ21, LMPT21]. **High** [BLB20, EVKL21, KUNT20, NBE<sup>+</sup>23, OKI<sup>+</sup>21, BSF20, DK23, GWN21, GVJ<sup>+</sup>22, KE23b, KGG21, KDP<sup>+</sup>22, LHC<sup>+</sup>21, MZ21, PPV<sup>+</sup>21, RD23, XLW<sup>+</sup>22]. **high-level** [BSF20]. **High-order** [EVKL21]. **High-performance** [BLB20]. **high-polarity** [DK23]. **high-speed** [GWN21]. **High-throughput** [NBE<sup>+</sup>23]. **Higher** [HFPS20]. **highest** [KPHV23, LJW<sup>+</sup>23]. **Highly** [JFZ<sup>+</sup>20, SHH<sup>+</sup>23b, SHH<sup>+</sup>23a]. **Hirshfeld** [LC22, MSE<sup>+</sup>21]. **histogram** [MT20b]. **HIV** [GG22, NPGP23, PWX<sup>+</sup>20, WCT<sup>+</sup>23]. **HIV-1** [PWX<sup>+</sup>20, WCT<sup>+</sup>23]. **HMX** [ZG21]. **Hoff** [ZXD20b, ZXD20a]. **Hoff/Le** [ZXD20b, ZXD20a]. **Hole** [RZS<sup>+</sup>23, JGGPN21, LK22, Sch22a, SJZ<sup>+</sup>21].

**HOMO** [CMD<sup>+</sup>22]. **HOMO-LUMO** [CMD<sup>+</sup>22]. **homodimeric** [DPSG20]. **homology** [CFOMCB<sup>+</sup>22]. **Homolytic** [LR20]. **hoops** [FDD<sup>+</sup>23]. **HOPO** [SDK20]. **Hopping** [YXGZ20, FCPG20]. **host** [BRNB21, GBM20, MJS<sup>+</sup>23, PPRS22, YLZ<sup>+</sup>22]. **host-guest** [BRNB21, GBM20, MJS<sup>+</sup>23, YLZ<sup>+</sup>22]. **hosts** [KPKS23]. **hot** [KSS21b, KSRB<sup>+</sup>21]. **HRas** [XZX<sup>+</sup>22]. **Hubbard** [POPGS22, TLD<sup>+</sup>22]. **huge** [JKK<sup>+</sup>21]. **Human** [KUNT20, KLZ<sup>+</sup>23, LSC<sup>+</sup>23, SCCZ21]. **human-norovirus** [LSC<sup>+</sup>23]. **Hybrid** [CdSB<sup>+</sup>21, ZK21, AR20, BOPJ<sup>+</sup>21a, FV20, HUUO23, KGS<sup>+</sup>21, MN20, MKK<sup>+</sup>22, NG20, RPD<sup>+</sup>20a, SS20, SZP<sup>+</sup>20, WKD<sup>+</sup>21, XZW<sup>+</sup>21, YW20]. **hybrids** [CPG21, HSG21, OMC<sup>+</sup>20]. **hydrate** [MJS<sup>+</sup>23]. **hydrated** [YC20]. **hydrates** [VCRP23]. **Hydration** [ALA<sup>+</sup>22, HS22, KPTT21, PCI23, KK23, TTK23, YIO20]. **hydrazine** [PFP<sup>+</sup>21]. **Hydrides** [PWW20]. **hydrocarbon** [NS22]. **hydrocarbons** [GAP21]. **Hydrocyanation** [JFZ<sup>+</sup>20]. **Hydrogen** [HS23, SKKG22, AV20, ARR22b, AD23, BCN22, CVGVN<sup>+</sup>20, CL23, CB20, DHN<sup>+</sup>21, DLH<sup>+</sup>23, GJL21, GH22b, KPTT21, LKT21, NTK21, SGGG22, SS23, SJZ<sup>+</sup>21, SD21, TTT<sup>+</sup>21, ZFRM20]. **hydrogen/halogen** [SJZ<sup>+</sup>21]. **hydrogenation** [ZZG<sup>+</sup>21]. **hydrolysis** [ZLLL22]. **hydrophilicity** [MSA22a]. **hydrophobic** [KPKS23]. **Hydrostatic** [SL20]. **hydroxochromones** [AIV20]. **hydroxylation** [HYA<sup>+</sup>20, MNH21]. **hydroxymethyl** [MSA22a]. **hydroxyquinolinato** [AS20]. **hydroxyquinolinone** [SEBE21]. **hyper** [MAI22]. **hyper-softness** [MAI22]. **hypercoordinate** [YrYqLhC23]. **Hypercube** [Bal20a]. **hypericin** [DMTR22]. **Hyperplanes** [Bal20a]. **hypervalent** [SCZ<sup>+</sup>21].

**I/II** [RLHG<sup>+</sup>23]. **icosahedral** [PGP<sup>+</sup>23]. **idea** [BBB<sup>+</sup>23]. **Identification** [PPP21, RDK<sup>+</sup>22, LCP21, MSE<sup>+</sup>21]. **identified** [SSYB<sup>+</sup>20]. **identify** [KDP<sup>+</sup>22, LKK<sup>+</sup>23, Sch22b, SYS<sup>+</sup>21, WRVP22]. **Identifying** [PAS<sup>+</sup>20]. **IGMP** [LKK<sup>+</sup>23]. **II** [ABZ20b, AD20, GP21, SVDS21, SSS<sup>+</sup>20a, YYS20, GH22a, RLHG<sup>+</sup>23]. **III** [AS20, HRTSS<sup>+</sup>20, KKAK23, RLHG<sup>+</sup>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<sup>+</sup>21b, BOPJ<sup>+</sup>21b, CX21a, ETT21a, GPM21a, GKA<sup>+</sup>23a, KFTB20a, KSS21a, KK22b, MLG<sup>+</sup>21a, QLW<sup>+</sup>22a, RPD<sup>+</sup>20b, SWM<sup>+</sup>20a, dRHB21, SSFS22a, TTH<sup>+</sup>21b, TCS<sup>+</sup>21b, VV20a]. **images** [QLW<sup>+</sup>22b]. **Imidazole** [CFOMCB<sup>+</sup>22]. **imidazopyridine** [ZOD<sup>+</sup>22]. **imino** [YFS20]. **immersive** [MSL<sup>+</sup>20]. **Immunodeficiency** [KUNT20]. **impact** [KDKS21, OM23, SPSH20, VCRP23]. **impacts** [MVV22]. **Implementation** [HAC<sup>+</sup>23b, NP23, YLZ<sup>+</sup>20, CSGVF<sup>+</sup>20, CPG21, FR21, OMC<sup>+</sup>20, SSDL<sup>+</sup>23]. **implementations** [CHVF21]. **implications** [KSP21]. **Implicit**

[GRBN21, GCL<sup>+</sup>20, CCHS23, RPD<sup>+</sup>20a]. **Importance** [HKS<sup>+</sup>20, DSB23]. **important** [SGGG22]. **improbability** [RLR<sup>+</sup>20]. **Improved** [BBK20, LJ20, CX21b, DKB23, RTB<sup>+</sup>22, ZKJ<sup>+</sup>23]. **Improving** [FB20, MKK<sup>+</sup>22, PNT<sup>+</sup>22, SZP<sup>+</sup>20, YFH<sup>+</sup>21, FYIO23]. **in-situ** [WKG<sup>+</sup>23]. **includes** [VWJ23]. **including** [FBP<sup>+</sup>22]. **inclusion** [YLZ<sup>+</sup>22]. **incorporating** [Gie21]. **incorrectly** [GAP21]. **increase** [LKM20]. **increases** [HREvdK<sup>+</sup>20]. **Independent** [LC22, CSG<sup>+</sup>21, LGC21, WFBB22]. **index** [PC23, Sch22b]. **Indexes** [WZZ<sup>+</sup>20, KdILC22]. **individual** [AD23, BRNB21]. **INDO** [Gie21]. **INDO/S** [Gie21]. **Induced** [QB20, EK20b, EK20c, FVSS20, KK22c, SCC<sup>+</sup>22, TTH<sup>+</sup>21a]. **inexpensive** [Ben22]. **Influence** [GAG20, MCP23, PT21, SGGG22, Brz22, CCHS23, SVDS21]. **influenza** [SSS<sup>+</sup>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, 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, 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, Ano23-27, Ano23b, Ano23c, Ano23d, Ano23e, Ano23f, Ano23g, Ano23h, Ano23i, Ano23j, Ano23k, Ano23l, Ano23m, Ano23n, Ano23o, Ano23p, Ano23q, Ano23r, Ano23s, Ano23t, Ano23u, Ano23v, Ano23w, Ano23x, Ano23y, Ano23z, TAC<sup>+</sup>23]. **information-theoretic** [TAC<sup>+</sup>23]. **infrared** [GPEK<sup>+</sup>20, KGS<sup>+</sup>22, LZW<sup>+</sup>23, PGP<sup>+</sup>21]. **Ingenuity** [FYIO23]. **ingredients** [MBBU23]. **inhibition** [dSCCN21, YC23]. **inhibitor** [BAO<sup>+</sup>20, BVC<sup>+</sup>23, EIT<sup>+</sup>21, GG22, MIK<sup>+</sup>23]. **inhibitors** [CFOMCB<sup>+</sup>22, KGD<sup>+</sup>21, MPuS<sup>+</sup>20, PWX<sup>+</sup>20, PPP21, PPRS22, RKC21, RDK<sup>+</sup>22, SKL23, TWT<sup>+</sup>22, ZOD<sup>+</sup>22]. **inhibitory** [BHR<sup>+</sup>21]. **inhibits** [HTFY21]. **initial** [AAID22]. **Initio** [SK20, VAL20, BSS<sup>+</sup>22, BBC<sup>+</sup>21a, DC22b, FCB23, GP21, KPTT21, Kop22a, KGD<sup>+</sup>21, MAM<sup>+</sup>23, MN20, PGP<sup>+</sup>23, RZS<sup>+</sup>23, RPD<sup>+</sup>20a, dASRHB21, SPSH20, SNN<sup>+</sup>21, XSP<sup>+</sup>23, KRSD<sup>+</sup>23]. **inner** [Sán20]. **inner-shell** [Sán20]. **inorganic** [Brz22, KGS<sup>+</sup>21, KS21, SZP<sup>+</sup>20]. **input** [GSD<sup>+</sup>22, VAP<sup>+</sup>21]. **inputs** [HREvdK<sup>+</sup>20]. **inserted** [LZW<sup>+</sup>23]. **Insight** [JFZ<sup>+</sup>20, KPHV23, MK22b, DGM22, HRTSS<sup>+</sup>20, YJZ<sup>+</sup>22]. **Insights** [ASL<sup>+</sup>20, BRNB21, FLT23, GOY20, MNH21, SAZ<sup>+</sup>23, SZP<sup>+</sup>20, CP23, KFLP21, MML<sup>+</sup>23, PPRS22]. **inspired** [MSA22a]. **Instanton** [SRB21]. **insulator** [EK20b]. **insulator-to-metal** [EK20b]. **integral**

[Gao20, Nee23, SCvW22, Shi22]. **integrals** [DWZ22, IN23a, IN23b]. **Integrated** [BBB<sup>+</sup>23, VDK<sup>+</sup>20, MLG<sup>+</sup>21b, SWLC22]. **Integration** [VWFR21, KCGK20]. **intelligence** [DPY<sup>+</sup>22]. **intensities** [TTT<sup>+</sup>21]. **intensity** [GAP21]. **inter** [BOPJ<sup>+</sup>21a]. **inter-molecular** [BOPJ<sup>+</sup>21a]. **interacting** [CSGVF<sup>+</sup>20, JCMHT22, JGGPN21, OE20, TPZ<sup>+</sup>20]. **Interaction** [KUNT20, MBBU23, PT20, dCRM21, AA20, ASW20, BdLC21, CV22, CSWW20, COK22, GKO<sup>+</sup>22, HTFY21, IN23a, Jab22b, KWYN23, KLZ<sup>+</sup>23, MAM<sup>+</sup>23, MR21, MPR22, MEKH22, NI22, PHS<sup>+</sup>20, QLW<sup>+</sup>22b, TWT<sup>+</sup>22, TTK23, VCRP23, WMZJ20, WKL22, YOCMA23, YLZ<sup>+</sup>22]. **interaction-site** [KWYN23]. **Interactions** [BWM20, LJ20, WP20, BW22a, BS23, BRNB21, BPDG21, CM20b, CTBB20, EPT21, FDD<sup>+</sup>23, FM21, HPG20, HTFY21, Klo22, KKAK23, KGD<sup>+</sup>21, LKK<sup>+</sup>23, LEP<sup>+</sup>21, LC22, MJS<sup>+</sup>23, ODL20, OE20, PDC23, RZS<sup>+</sup>23, RMJ21, SAZ<sup>+</sup>23, SI22, YW20]. **Interatomic** [AA20, ZFRM20]. **intercalation** [HKS20, SGGG22]. **interesting** [HPG20]. **interface** [ABNG22, DMD<sup>+</sup>21, SNN<sup>+</sup>21]. **interfacial** [CM20a]. **intermediate** [MMK<sup>+</sup>20]. **Intermediates** [SK20, DSB23, LHG<sup>+</sup>23]. **Intermolecular** [KGD<sup>+</sup>21, Ooy20, BSS<sup>+</sup>22, HTFY21, LLZ<sup>+</sup>23, MGCM21, RZS<sup>+</sup>23, SI22]. **Internal** [WZZ<sup>+</sup>20, ABTM22, BLB20, KZJ22]. **Interplay** [HYA<sup>+</sup>20, ZRSST20]. **Interpolation** [WSL<sup>+</sup>20, GWN21]. **interpretable** [BK22]. **Interpretation** [LCC<sup>+</sup>21]. **interpreter** [PSGL21]. **intersection** [AIV20]. **Interstitial** [PGP<sup>+</sup>21]. **intra** [BOPJ<sup>+</sup>21a]. **intra-** [BOPJ<sup>+</sup>21a]. **Intramolecular** [FM21, ARR22b, AIV20, CRT<sup>+</sup>21, FP22, KSP21, RA20]. **Intrinsic** [AD20]. **intrinsically** [SY21]. **Introducing** [SKS21]. **invariant** [KSRB<sup>+</sup>21, OKK22]. **inverse** [LBH<sup>+</sup>22]. **inversion** [SWF<sup>+</sup>20, SWM<sup>+</sup>20b]. **Investigating** [BSL20]. **Investigation** [CSP20, ČPP<sup>+</sup>22, DOT22, HL20, AQMM<sup>+</sup>23, DHN<sup>+</sup>21, FBM<sup>+</sup>23, KPTT21, KDKS21, KJV23, KK22a, MKB<sup>+</sup>21, NMMC21, SS20, SKGG23, ZS22]. **investigations** [RZS<sup>+</sup>23]. **involved** [CRT<sup>+</sup>21]. **Involving** [SK20, KZJ22, SJZ<sup>+</sup>21, SBB<sup>+</sup>22, ZBH<sup>+</sup>23]. **IOData** [VAP<sup>+</sup>21]. **Iodido** [SVDS21]. **Iodine** [ASL<sup>+</sup>20, DMTR22, SCZ<sup>+</sup>21]. **iodine-containing** [DMTR22]. **Iogansen** [TTT<sup>+</sup>21]. **Ion** [SLR<sup>+</sup>20, CX21b, FVSS20, HPG20, JRS20, LA20, OM23, XAD20, YJZ<sup>+</sup>22]. **ion-induced** [FVSS20]. **Ion-Pair** [SLR<sup>+</sup>20]. **Ionic** [VAL20, AÅFJ21, Cer22, LWF<sup>+</sup>22, LEP<sup>+</sup>21, SI22, XAD20]. **ionization** [ALA20, MLB<sup>+</sup>23]. **ions** [KEK23, ODL20, SDK20, YC20]. **IR** [TTT<sup>+</sup>21, DZL<sup>+</sup>20]. **iron** [CL23, GKA<sup>+</sup>23b, Jab22b, KKAK23, SHP<sup>+</sup>23]. **irradiation** [LYX<sup>+</sup>22]. **Irreducible** [Bal20a]. **isodesmic** [WKCP21]. **isodesmic-type** [WKCP21]. **Isoelectronic** [ZXD20a, SVTK<sup>+</sup>22, SK23, ZXD20b]. **isolable** [FNPD22]. **isolated** [CA22, IW23, JS21, LML<sup>+</sup>23]. **Isolation** [BLP20, LRKD23]. **isoleucine** [MPOC21]. **isomerase** [DPSG20]. **isomerization** [OKI<sup>+</sup>21]. **isomers** [OKI<sup>+</sup>21, ONC20]. **isothermal** [LL21a]. **isotope** [JMK<sup>+</sup>20, dCVERN20]. **isotopologues** [SR23]. **iSPECTRON** [SNN<sup>+</sup>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, Ano23-27, Ano23b, Ano23c, Ano23d, Ano23e, Ano23f, Ano23g, Ano23h, Ano23i, Ano23j, Ano23k, Ano23l, Ano23m, Ano23n, Ano23o, Ano23p, Ano23q, Ano23r, Ano23s, Ano23t, Ano23u, Ano23v, Ano23w, Ano23x, Ano23y, Ano23z, RPD+20b]. **iterative** [VV21]. **IV** [CMD+22, PPSP20, SVDS21].

**J** [MT20a, WG21]. **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]. **Key** [VV20b, FM21, PPRS22, TANC23]. **kinase** [SNW22, TWT+22]. **kinase-2** [TWT+22]. **kinematic** [HC21]. **kinetic** [EG20, JMK+20, MIK+23, WKG+23, dCVARN20]. **Kinetics** [SK20, CGMRVBAl22, CD20, DWSX20, RMJ21, SNW22, ZLLL22]. **kinks** [MA23b]. **Kohn** [BTSB22, EK20a, HCS+20, MB21]. **Koopmans** [GX20]. **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]. **landscape** [BBC20, SY21, YYS20]. **landscapes** [GVJ+22, PPV+21]. **Langevin** [SH23]. **Lantern** [LLKS23]. **Lantern-type** [LLKS23]. **lanthanides** [ALA+22, SLB23]. **Laplacian** [TTDT20]. **Large** [MFC20, NS22, UAC+23, AD23, CJHW21, JKS23, KS21, RBM+23, SSDL+23]. **large-scale** [CJHW21]. **Large-Sized** [MFC20]. **laser** [LYX+22, LAM+23, SCC+22]. **laser-induced** [SCC+22]. **Late** [PWW20]. **lattice** [NMF121]. **layer** [YrYqLhC23]. **layered** [EK20c]. **layers** [LMPT21]. **lead** [AQMM+23]. **lead-free** [AQMM+23]. **Leading** [AD20, NG20]. **leapfrog** [MIP+21]. **Learning**

[LPP20, BP22, CdSB<sup>+21</sup>, COK22, HBT<sup>+20</sup>, JGK<sup>+22</sup>, KM22, KB22, KDP<sup>+22</sup>, MLC<sup>+23</sup>, NGD22, RDB23, SKL23, TCS<sup>+21a</sup>, WRBT21, WLSC23a, YFS20]. **learning-assisted** [WRBT21]. **length** [FR21, MVP<sup>+20</sup>]. **Lennard** [SG20]. **Lennard-Jones** [SG20]. **less** [CSWW20]. **leucine** [CGMRVBAI22]. **leucoindigo** [PPFL23]. **level** [ABNG22, BSF20, JK21, PHS<sup>+20</sup>]. **levels** [Kop22b]. **Lewis** [Brz23, FP22, NMMC21, OE20, PT21, PLZT23, ZS22]. **Li** [LEP<sup>+21</sup>]. **Libkrylov** [RBM<sup>+23</sup>]. **library** [JGK<sup>+22</sup>, KRSD<sup>+23</sup>, RBM<sup>+23</sup>, RDS<sup>+20</sup>, VAP<sup>+21</sup>, WHJM23]. **Lif** [VDK<sup>+20</sup>]. **lifetime** [FCB23]. **Ligand** [Ban20, JFZ<sup>+20</sup>, KW22, MXM20, NNT<sup>+20</sup>, AAe20, BKM21, HGF20, IK21, KDLP21, KK23, KDP<sup>+22</sup>, LYKS23, MAKZ23, Ngo21, ÖLP<sup>+20</sup>, OM23, PMT<sup>+22</sup>, PNT<sup>+22</sup>, PSB<sup>+22</sup>, SNW22, TWT<sup>+22</sup>, TTK23, VWP<sup>+22</sup>, WCD<sup>+23</sup>, YIO20, ZOD<sup>+22</sup>]. **ligand-alkali** [OM23]. **ligand-based** [PMT<sup>+22</sup>]. **Ligand-Binding** [NNT<sup>+20</sup>, HGF20, Ngo21]. **ligand-free** [YIO20]. **ligand-ranking** [PNT<sup>+22</sup>]. **Ligand-stabilized** [KW22]. **Ligands** [Min20, SZLD20, DDSM23, GPM21b, LLKS23, RvWH23, SVDS21, TLS23]. **lignin** [BW22a]. **like** [DYGM21, LSC<sup>+23</sup>, SAZ<sup>+23</sup>, YMSS23]. **limit** [CVGVN<sup>+20</sup>, SCKH21]. **limitations** [TZS<sup>+22</sup>]. **limits** [WFBB22]. **LIMONADA** [CBB<sup>+21</sup>]. **linear** [OKK22, Sch22a, SNN<sup>+21</sup>, Tou21]. **linearized** [NSRK21]. **link** [GH22a, KGTL21]. **linker** [GJL21]. **Links** [GFRNC21]. **LIO** [SDK20]. **Lipase** [VDK<sup>+20</sup>]. **lipid** [KFTB20b, WRBT21]. **lipids** [KCF<sup>+20</sup>]. **lipophilicity** [HS22]. **liquid** [KGS<sup>+22</sup>, LEP<sup>+21</sup>, SPSH20, ZWY<sup>+22</sup>]. **liquid-based** [LEP<sup>+21</sup>]. **Liquids** [VAL20, BUNO22b, Cer22, LWF<sup>+22</sup>, SI22, TPD21]. **lithium** [HM21, KE23b, Kop22b, Mil21, SGT<sup>+20</sup>]. **lithium-based** [HM21]. **lithium-chloride** [Mil21]. **LLS** [GKO<sup>+22</sup>]. **LLS-SC** [GKO<sup>+22</sup>]. **load** [DLH<sup>+23</sup>]. **LOBSTER** [NEG<sup>+20</sup>]. **Local** [NEG<sup>+20</sup>, PKT21, SPT21, WSV20, DTA21, FB21, FDK22, GFRNC21, MAI22, PW20, TV22, VV20b]. **localization** [BMT23, LT23, WFLZ23]. **localized** [CdSB<sup>+21</sup>]. **locating** [SDH23]. **logarithm** [SHH<sup>+23b</sup>]. **Lone** [TTDT20]. **Long** [BBK20, LSC<sup>+23</sup>, AS21, CHVF21, GAP21, HTFY21, HCS<sup>+20</sup>]. **Long-range** [BBK20, AS21, CHVF21, GAP21, HTFY21, HCS<sup>+20</sup>]. **Long-time** [LSC<sup>+23</sup>]. **look** [NSKN21]. **lookup** [GWN21]. **loop** [LLS22a]. **loops** [OC23]. **low** [BBY<sup>+21</sup>, CK22, IK21, LWLC21, MdSJ<sup>+23</sup>, OM23, SM22b]. **low-cost** [CK22]. **low-lying** [IK21, MdSJ<sup>+23</sup>]. **low-symmetry** [SM22b]. **Löwdin** [ASW20]. **lowest** [FCB23]. **LSL** [FR21]. **LSL-BFGS** [FR21]. **LSLOpt** [FR21]. **Lu** [SLB23]. **LUMO** [CMD<sup>+22</sup>]. **lutidine** [TYZ20]. **lying** [IK21, MdSJ<sup>+23</sup>].

**M** [AS20, HSG21, MH20, PPP21, ZMH<sup>+21</sup>, AS20, MH20, PTP23, PP23, ZMH<sup>+21</sup>]. **Machine** [MLC<sup>+23</sup>, CdSB<sup>+21</sup>, COK22, HBT<sup>+20</sup>, KM22, KB22, KDP<sup>+22</sup>, NGD22, RDB23, SKL23, TCS<sup>+21a</sup>, WRBT21, YFS20]. **Machine-learning** [MLC<sup>+23</sup>, KDP<sup>+22</sup>]. **Macroscale** [HZG<sup>+20</sup>]. **made** [TPD21]. **magnesium** [ZDBZ20]. **Magnetic**

[KKAK23, ABAQ<sup>+</sup>23, LL21b, SBFSJMLU23, TPD21]. **magnetizabilities** [SZL23]. **maiden** [Jab22b]. **main** [Klo22, PPP21, RMJ21, UAC<sup>+</sup>23, WCD<sup>+</sup>23, YC23]. **main-group** [Klo22, RMJ21, WCD<sup>+</sup>23]. **Mannose** [KUNT20]. **many** [BMT23, CN21, KSP21, NI22, WFLZ23]. **many-body** [BMT23, KSP21, NI22, WFLZ23]. **many-particle** [CN21]. **Map** [CLS<sup>+</sup>20]. **mapping** [TTDT20]. **Martini** [MT20a, MT21, BAC20, MT19]. **Massively** [BBK<sup>+</sup>21, ABTM22, JKS23]. **material** [GGK20, LHH<sup>+</sup>23, MMAZ<sup>+</sup>23, SPT21, SGT<sup>+</sup>20]. **materials** [LRF<sup>+</sup>21, LWLC21, PSGL21, SAZ<sup>+</sup>23, TV22, ZGZ<sup>+</sup>20]. **Mathematical** [QB20]. **Matrix** [BLP20, BBK<sup>+</sup>21, RBM<sup>+</sup>23, RA20, TT20, WMZJ20, WHJM23, XSP<sup>+</sup>23]. **matrix-product** [WMZJ20]. **Maximal** [Sch22a]. **maximum** [CTPJH22, TLD<sup>+</sup>22]. **MBAR** [JGM21]. **MBN** [SSFS22b]. **McConst** [SKS21]. **MCML** [BMT<sup>+</sup>21]. **MCO** [GPM21b]. **MD** [FCB23, FBP<sup>+</sup>22, HKFT21, SSS<sup>+</sup>20a, TTK23]. **MDMS** [Zac20]. **Me** [HSG21, SDK20, WLZM20]. **Me-3** [SDK20]. **Mean** [PPV<sup>+</sup>21]. **means** [DKB23, HRTSS<sup>+</sup>20]. **measure** [AA20]. **Mechanical** [SL20, AAe20, GPEK<sup>+</sup>20, HKS20, MMK<sup>+</sup>20, MMAZ<sup>+</sup>23, PWX<sup>+</sup>20, PGP<sup>+</sup>21, SPSH20]. **mechanics** [BRNB21, CLTMd<sup>+</sup>23, DC22b, FDK22, KGD<sup>+</sup>21, TCS<sup>+</sup>21a]. **mechanics/molecular** [CLTMd<sup>+</sup>23, FDK22]. **Mechanism** [Ban20, CWZD20, WLZM20, ZZ23b, ABZ20b, CJHW21, CD20, CSP20, CRT<sup>+</sup>21, DOT22, GPM21b, HRTSS<sup>+</sup>20, KZJ21, KR23, KSS21b, LRqG<sup>+</sup>22, LBH<sup>+</sup>22, MNH21, MIP<sup>+</sup>22, NMCM21, NST<sup>+</sup>20, PPSP20, PM21, SVDS21, SMB<sup>+</sup>23, SKGG23, SCZ<sup>+</sup>21, YC23]. **mechanism-enabled** [LBH<sup>+</sup>22]. **Mechanisms** [CGMRVBAl22, BCN22, LA20, LEP<sup>+</sup>21, MNZGO<sup>+</sup>20, NYM22, ONA<sup>+</sup>20, PC21, SWF<sup>+</sup>20, SWM<sup>+</sup>20b, ZLLL22]. **Mechanistic** [AMM22, HCY<sup>+</sup>22, JFZ<sup>+</sup>20, KZJ22, PPRS22, TYZ20, ZMH<sup>+</sup>21, ARA22, LGJF22]. **mechanistically** [KCF<sup>+</sup>20]. **mediated** [JGSA22, SKGG23, TYZ20]. **medicinal** [BBB<sup>+</sup>23, TCS<sup>+</sup>21a]. **medium** [BSS<sup>+</sup>22, GH22b, LSP23, LRKD23, PDC23, YC20]. **medium-resolution** [LSP23]. **melting** [CST23]. **melts** [WKD<sup>+</sup>21]. **membered** [DSB23, KZJ22]. **Membership** [GJMPB<sup>+</sup>20]. **Membrane** [BWM20, FMFG20, HHL<sup>+</sup>20, KCF<sup>+</sup>20, VDK<sup>+</sup>20, CX21b, IBL20, NLC23, ZSD<sup>+</sup>20]. **Membrane-Integrated** [VDK<sup>+</sup>20]. **Membranes** [PT20, AAID22, CBB<sup>+</sup>21, MSA22a, WRBT21]. **mer** [HHL<sup>+</sup>20, LGD<sup>+</sup>20]. **mercaptapurine** [NST<sup>+</sup>20]. **mercury** [LGD<sup>+</sup>20, MDO<sup>+</sup>20]. **Merocyanine** [TMO<sup>+</sup>21]. **mesh** [RCC21]. **mesophilic** [NYM22]. **meta** [BMT<sup>+</sup>21, NG20]. **meta-generalized** [BMT<sup>+</sup>21]. **meta-generalized-gradient** [NG20]. **Metadynamics** [Tik23, KN21, KSRB<sup>+</sup>21, LL21a, NN20, PPSP20, TM20]. **Metal** [HHL<sup>+</sup>20, PWW20, AR20, AS23, BKM21, DGM22, DOT22, EK20b, FBM<sup>+</sup>23, HRTSS<sup>+</sup>20, IK21, JMV21, MAM21, MAI22, MCD22, NBE<sup>+</sup>23, OM23, OSM20, PTP23, PDGD23, PSM<sup>+</sup>20, POPGS22, TYZ20, WP20, YFS20, YMSS23, ZBH<sup>+</sup>23, dBCdL20]. **metal-dinitrogen** [DGM22].

**metal-doped** [DOT22]. **metal-free** [TYZ20]. **metal-involving** [ZBH<sup>+</sup>23].  
**metal-ligand** [BKM21]. **metal-organic** [HRTSS<sup>+</sup>20, MAM21, WP20].  
**metal-to-ligand** [IK21]. **metal/** [AR20]. **metallic** [CBF<sup>+</sup>20]. **metallo**  
 [KGD<sup>+</sup>21]. **metallo-** [KGD<sup>+</sup>21]. **metallocenes** [HSG21]. **metallofullerenes**  
 [DA22]. **metals** [PTP23, VV20b]. **metastability** [SMH21]. **methacrylate**  
 [MSA22a]. **methane** [DZL<sup>+</sup>20, IMT<sup>+</sup>21]. **methanol**  
 [DHN<sup>+</sup>21, RPD<sup>+</sup>20a, SSM21]. **Method** [QB20, AD23, AKN<sup>+</sup>20, ABTM22,  
 AYO20, AiIS<sup>+</sup>21, BBK<sup>+</sup>21, CK22, DWSX20, Dor20, EK20a, EVKL21, Fed22,  
 FBP<sup>+</sup>22, HKFT21, HTFY21, IYI<sup>+</sup>20, IN23a, JGM21, LWF<sup>+</sup>22, LRqG<sup>+</sup>22,  
 LC22, MMK<sup>+</sup>20, MA23a, MA23b, MT20b, MSS20, NAN<sup>+</sup>23, PDL<sup>+</sup>21,  
 PSMPB21, RSHG23, SS20, SDH23, SKKK20, SHH<sup>+</sup>23b, SHH<sup>+</sup>23a,  
 TTH<sup>+</sup>21a, WKG<sup>+</sup>23, YLZ<sup>+</sup>20, YAO20, ZK21, ZLLL22]. **method-based**  
 [ZLLL22]. **Methods**  
 [AWID<sup>+</sup>20, KUNT20, PAS<sup>+</sup>20, SK20, ASW20, BSF20, BF22, CTPJH22, FB21,  
 GUCCR20, KRSD<sup>+</sup>23, KB22, NBE<sup>+</sup>23, OM22, PW20, PB20, RLHG<sup>+</sup>23,  
 RvWH23, SW21, SYS<sup>+</sup>21, SM22a, SC22, Sts20, SHH<sup>+</sup>23b, SHH<sup>+</sup>23a, TZS<sup>+</sup>22].  
**methotrexate** [PRH20]. **methotrexate-camptothecin** [PRH20].  
**methoxyethyl** [MSA22a]. **methyl** [PGP<sup>+</sup>23, SKGG23]. **methyllide**  
 [SVTK<sup>+</sup>22]. **Metropolis** [EG20]. **Mg**  
 [SM22b, DSC20, GP21, JRS20, ZRSST20, ZDBZ20]. **MgCl** [AMM22]. **MgO**  
 [DA22]. **micellization** [ZK21]. **microhydrated** [GJL21]. **microkinetic**  
 [CJHW21, SC23]. **Microscale** [HZG<sup>+</sup>20]. **Microscopic** [PT20].  
**microsolvated** [OM22]. **microsolvation** [STR20]. **MIDAS** [GJMPVR<sup>+</sup>20].  
**midbond** [MEKH22]. **milder** [GM22]. **mimetic** [HTFY21]. **Minimal**  
 [HHL<sup>+</sup>20, JGGPN21]. **minimize** [AiIS<sup>+</sup>21]. **minimizing** [YBS<sup>+</sup>20].  
**minimum** [DC22a, RH21, SDH23]. **Mixed** [CDCT21]. **Mixed-solvent**  
 [CDCT21]. **mixture** [NS22]. **MkVsites** [LKM20]. **ML** [TTK23]. **MLLPA**  
 [WRBT21]. **MM**  
 [ABNG22, BBC20, GH22a, LRqG<sup>+</sup>22, Mar21, PCI23, SSS<sup>+</sup>20a, SHH<sup>+</sup>23b].  
**MM-PBSA** [SHH<sup>+</sup>23b]. **MNDO** [FCB23]. **MNDO-MD** [FCB23]. **Mo**  
 [MAM21]. **Mo-Oxo** [MAM21]. **mobilities** [LHC<sup>+</sup>21]. **MoBioTools**  
 [CLTMd<sup>+</sup>23]. **MOCASSIN** [EG20]. **mode** [FDK22, San21, SH23]. **Model**  
 [GCL<sup>+</sup>20, HRT<sup>+</sup>20, LGM20, MT20a, SSS<sup>+</sup>20a, BW22a, BPDG21, CC22,  
 CX21b, CQSG20, DKB23, GSH23, Gie21, HKSW20, HPG20, IN23b, IK21,  
 KWYN23, KdILC22, KPKS23, LC22, MDO<sup>+</sup>20, MT19, MGCM21, NGD22,  
 RPD<sup>+</sup>20a, SWF<sup>+</sup>20, SWM<sup>+</sup>20b, SSO<sup>+</sup>20, SHH<sup>+</sup>23a, TLD<sup>+</sup>22, UB20, VL22,  
 VAL20, VFCG20, WKL22, XAD20]. **model-compounds** [BW22a].  
**model/energy** [MGCM21]. **modeler** [SKS21]. **Modeling**  
 [AWID<sup>+</sup>20, BLP20, BS23, FVSS20, GNK<sup>+</sup>23, KDLP21, KB22, LJ20,  
 LWLC21, LDT<sup>+</sup>22, PAF<sup>+</sup>20, SHM<sup>+</sup>20, ZOD<sup>+</sup>22, BHR<sup>+</sup>21, CFOMCB<sup>+</sup>22,  
 COK22, GWN21, GUCCR20, KGTL21, Kos22, LLS22a, LGD<sup>+</sup>20, LL21b,  
 LL22, MGB<sup>+</sup>22, MZ21, MSA22b, PSGL21, SSFS22b]. **models**  
 [AVM21, BK22, BSR22, BP22, CCHS23, CTBB20, HPM<sup>+</sup>21, JGGPN21,  
 KK23, KOD21, LGJF22, LBH<sup>+</sup>22, LMPT21, MK22a, PLP<sup>+</sup>20, PMT<sup>+</sup>22,

PCI23, SKL23, UB20, WP20]. **modes** [CBF<sup>+</sup>20, dBCdL20]. **Modification** [AWID<sup>+</sup>20, Ban20]. **Modified** [SG20, DOT22, XAD20]. **Modifying** [PFPD21]. **modular** [RBM<sup>+</sup>23]. **Modulation** [ZSD<sup>+</sup>20]. **module** [WRBT21, WLSC23a]. **MOF** [FP23]. **moiety** [KPTT21]. **Molecular** [ARR22b, BCN22, CA22, FBM<sup>+</sup>23, FMFG20, GJMPB<sup>+</sup>20, GGK20, GCL<sup>+</sup>20, JRS20, KR23, KUNT20, MPOC21, MSA22a, NLC23, WCT<sup>+</sup>23, YXGZ20, Zac20, AV20, ARR22a, AD23, AKN<sup>+</sup>20, AAL21, AÁFJ21, AiIS<sup>+</sup>21, AS20, ALA<sup>+</sup>22, AMF<sup>+</sup>20, BUNO22b, BdLC21, BRNB21, BAO<sup>+</sup>20, BOPJ<sup>+</sup>21a, BP22, CFOMCB<sup>+</sup>22, CLTMd<sup>+</sup>23, CDCT21, CX23, CSP20, CMD<sup>+</sup>22, CST23, DO20, DHN<sup>+</sup>21, DHD21, EVKL21, Fed22, FDK22, FNY21, Gao20, GJMPVR<sup>+</sup>20, GG22, GSJ<sup>+</sup>23, HS23, HGF20, HPM<sup>+</sup>21, JKK<sup>+</sup>21, KZJ21, KG23, KK23, KLP<sup>+</sup>22, KPHV23, KGD<sup>+</sup>21, LL21a, LKM20, LHH<sup>+</sup>21, LKK<sup>+</sup>23, LKT21, LEP<sup>+</sup>21, LAM<sup>+</sup>23, MN20, MKK<sup>+</sup>22, MGB<sup>+</sup>22, MK22a, MAP<sup>+</sup>20, NAN<sup>+</sup>23, NI22, NGD22, NN20, NP23, OSHT20, PBM21, PDL<sup>+</sup>21, POvG21, PPP21, PL22, PSB<sup>+</sup>22, PM21, QLC<sup>+</sup>20, RKC21, RDK<sup>+</sup>22, RGGD21, RPD<sup>+</sup>20a, RDB23, RDS<sup>+</sup>20, SPSH20, SIW21, SYS<sup>+</sup>21, SAZ<sup>+</sup>23]. **molecular** [SCvW22, SKL23, Shi22, SY21, SWLC22, SMB<sup>+</sup>23, SKKK20, SZL23, SCCZ21, TWT<sup>+</sup>22, TPB22, TCS<sup>+</sup>21a, TSR21, UKBD23, WFBB22, WK21, WKL22, WKD<sup>+</sup>21, YGG<sup>+</sup>23, YC23, YrYqLhC23, ZK21, ZG21, ZWR22, ZZ23a, ZFRM20, KZJ22]. **molecular-dynamics** [UKBD23]. **molecular-orbital** [KK23]. **molecular-wide** [BdLC21]. **molecule** [AK20, GFRNC21, KFTB20b, SKL23, TANC23, YIO20, ZK23]. **Molecules** [LPP20, APS20, AG21, AZKM22, AA20, BGS<sup>+</sup>20, CKH23, CdSB<sup>+</sup>21, FB20, GGK20, GP21, Jab22b, KZOV23, KPR23, KdILC22, KPHV23, KYM20, LPF<sup>+</sup>23, LGM20, LGM22, LK22, LT23, LYX<sup>+</sup>22, LJW<sup>+</sup>23, MPP23, MC23, MLP22, MB21, NTK21, PFP<sup>+</sup>21, SRB21, Sch22a, Sch22b, SCC<sup>+</sup>22, SSO<sup>+</sup>20, SHH<sup>+</sup>23b, TIK21, TMO<sup>+</sup>21, TSR21, VCL20, WLWR22]. **molecules-in-molecules** [TSR21]. **Møller** [CSGVF<sup>+</sup>20, FKT21, Sán20]. **Møller-Plesset** [CSGVF<sup>+</sup>20, Sán20]. **MolSpin** [GNK<sup>+</sup>23]. **moments** [BSF20, LRKD23]. **Momentum** [FNY21, MR21]. **Mono** [ZXD20b, ZXD20a, HBM<sup>+</sup>20, MAKZ23]. **mono-** [MAKZ23]. **Mono-silicon** [ZXD20b, ZXD20a]. **monodentate** [TLS23]. **monolayers** [LHC<sup>+</sup>21, MMAZ<sup>+</sup>23]. **monomer** [ZLLL22]. **monooxygenase** [HYA<sup>+</sup>20]. **Monte** [DMD<sup>+</sup>21, EG20, GGK20, GNL<sup>+</sup>22, KCGK20, KEK23, PFSC20, TIK21, TMO<sup>+</sup>21, ZKJ<sup>+</sup>23]. **Monte-Carlo** [GNL<sup>+</sup>22]. **MonteCarbo** [AG21]. **MoO** [SM22b]. **moon** [HBM<sup>+</sup>20]. **MOPAC** [Gie21]. **MoSDeF** [DMD<sup>+</sup>21]. **motif** [HS23]. **motifs** [HC21, YrYqLhC23]. **motions** [BBSFA22, San21]. **MP** [ABTM22]. **MP2** [KG23, MEKH22, SW21]. **MP2/CCSD** [KG23]. **MPI** [AiIS<sup>+</sup>21]. **MRCI** [ZRSST20]. **MSMS** [WK21]. **Mukaiyama** [LLS<sup>+</sup>22b]. **Multi** [HREvdK<sup>+</sup>20, AS23, BBB<sup>+</sup>23, BMT<sup>+</sup>21, PMT<sup>+</sup>22, SY21, VM23]. **multi-decker** [AS23]. **multi-parametric** [PMT<sup>+</sup>22]. **multi-purpose** [BMT<sup>+</sup>21]. **multi-reference** [VM23]. **Multi-scale** [HREvdK<sup>+</sup>20, SY21]. **multi-use** [BBB<sup>+</sup>23]. **multicanonical** [BAO<sup>+</sup>20]. **multiconfigurational** [HRTSS<sup>+</sup>20, TT20]. **multicore** [GJMPVR<sup>+</sup>20]. **multideterminant**

[KRS<sup>D</sup>+23]. **multidimensional** [BCN22, GWN21]. **multifunctionalized** [AG21]. **multilayer** [IRB<sup>+</sup>23]. **multilevel** [SW21]. **Multilinear** [WSL<sup>+</sup>20]. **Multimolecular** [GP21]. **Multiple** [SZLD20, MKK<sup>+</sup>22, POvG21, WCT<sup>+</sup>23, XAD20]. **multiple-time-step** [POvG21]. **Multipolar** [HRT<sup>+</sup>20, YFH<sup>+</sup>21]. **multipole** [AYO20, AiIS<sup>+</sup>21, MSS20, YAO20]. **multipurpose** [TSZ<sup>+</sup>21]. **multireference** [SD21]. **Multiscale** [SSFS22b, FLT23, LGD<sup>+</sup>20, LGC21, Mar21]. **mussel** [MSA22a]. **mussel-inspired** [MSA22a]. **mutant** [BK22, CSP20]. **mutations** [HB21]. **Mycobacterium** [RDK<sup>+</sup>22].

**n** [ZDBZ20, ARR22b, BSS<sup>+</sup>22, DZL<sup>+</sup>20, GKA<sup>+</sup>23b, JGSA22, MKSS20, PAS<sup>+</sup>20, RC22, XLW<sup>+</sup>22, TTK23]. **N-co-doped** [DZL<sup>+</sup>20]. **N-heterocycles** [BSS<sup>+</sup>22]. **N-heterocyclic** [JGSA22]. **N-Terminal** [MKSS20]. **NADH** [CFOMCB<sup>+</sup>22]. **NADH-fumarate** [CFOMCB<sup>+</sup>22]. **NADP** [CWZD20]. **NADPH** [CWZD20]. **named** [SS20]. **nano** [FDD<sup>+</sup>23]. **nano-hoops** [FDD<sup>+</sup>23]. **nanobelts** [AS21]. **nanoclusters** [GAG20, MK22b]. **nanocrystals** [KPR23, Mil21]. **nanodiamonds** [KPDB22]. **nanometer** [NAAP21]. **nanoparticle** [LBH<sup>+</sup>22]. **nanoparticles** [BA22]. **nanopores** [YC20]. **nanoreactor** [FP23]. **nanoribbons** [SPT21]. **nanoring** [YLZ<sup>+</sup>22]. **nanoscale** [SG20]. **NanoShaper** [WK21]. **nanotube** [APS20, CTBB20]. **Nanotubes** [DBE20, BW22a, CBF<sup>+</sup>20, VCL20]. **Naphthalene** [NRH<sup>+</sup>20]. **naphthyridine** [WCD<sup>+</sup>23]. **Natural** [KL20, CB20, GRBN21, MH20, PW20, Sch22b, SD21]. **Nature** [MVP<sup>+</sup>20, PDC23, WG21, BRNB21, BPDG21, FDD<sup>+</sup>23, HSG21, Jab22b, KSP21, MC23, MP23, NTK21, Wan21a, Wan21b, dARW<sup>+</sup>23]. **NaY** [NS22]. **NbGe** [TT20]. **NBO** [LGJF22]. **NbX** [ABAQ<sup>+</sup>23]. **NCF** [OE20]. **NE-RDFE** [MPP23]. **near** [IRB<sup>+</sup>23]. **needs** [NGD22]. **negative** [TAC<sup>+</sup>23]. **neighbor** [GKO<sup>+</sup>22]. **neon** [LZW<sup>+</sup>23]. **neopentane** [NS22]. **NeRF** [ABTM22]. **Nernst** [CX21b]. **net** [ÖLP<sup>+</sup>20]. **net-charge** [ÖLP<sup>+</sup>20]. **Network** [BSL20, KOD21, MZ21, MLP22, NGD22, RTB23, SSM21, TIK21]. **networks** [VFCG20]. **neural** [MZ21, MLP22, NGD22, TIK21]. **neuroglobin** [FDK22]. **Neutral** [LL21a, BGS<sup>+</sup>20, KPKS23, MCP23, MP23]. **Neutralizing** [KUNT20]. **NEVPT2** [CS20]. **Newton** [MT20b]. **Next** [AMF<sup>+</sup>20, LYX<sup>+</sup>22]. **Next-generation** [AMF<sup>+</sup>20]. **Ng** [APR21]. **NgX** [APR21]. **NH** [OE20, XZW<sup>+</sup>21, HS23, SLR<sup>+</sup>20]. **NHCs** [DSB23]. **Ni** [LXP<sup>+</sup>22, SM22b, PTP23]. **NIAS** [FPMD23]. **NIAS-Server** [FPMD23]. **nickel** [DSK21, LLKS23, ZZG<sup>+</sup>21]. **nickel-nickel** [LLKS23]. **nicotinic** [BRNB21]. **nitrate** [YC20]. **Nitreones** [PAS<sup>+</sup>20]. **nitriolotriacetate** [CL23]. **nitrite** [YC20]. **nitroalkenes** [KZJ22]. **nitrobenzaldehyde** [VM23]. **nitrocellulose** [ZLLL22]. **nitrogen** [JMV21, XZZ<sup>+</sup>20]. **nitrogen-rich** [JMV21]. **nitrogenase** [GKA<sup>+</sup>23b, WS21]. **nitroimidazole** [CFOMCB<sup>+</sup>22]. **nitronates** [KZJ22]. **nitroprop** [SMB<sup>+</sup>23]. **nitrosyl** [KK23]. **nitrous** [KZJ21]. **nitroxide** [MC23]. **NLi** [SKKG22]. **NMR**

[Ben22, FBP<sup>+</sup>22, LL22, MPOC21, MPV22, MCD22, Sai23, TTDT20].  
**NMR-data-assisted** [LL22]. **NN** [LPP20]. **NO** [OKI<sup>+</sup>21]. **noble**  
 [APR21, MSYS23, YMSS23]. **NOCV** [DGM22, GM22, GKA<sup>+</sup>23b, SBB<sup>+</sup>22].  
**Noggin** [CM20b]. **Non**  
 [GAP21, KE23b, BdLC21, LGJF22, MP23, TAC<sup>+</sup>23, VV21]. **non-aqueous**  
 [VV21]. **non-bonding** [MP23]. **non-classical** [BdLC21]. **non-iterative**  
 [VV21]. **non-negative** [TAC<sup>+</sup>23]. **Non-nuclear** [KE23b]. **non-thermal**  
 [LGJF22]. **nonadiabatic** [SWM<sup>+</sup>20b]. **nonaqueous** [RPD<sup>+</sup>20a].  
**noncovalent**  
 [BW22a, CSWW20, CTBB20, OE20, OM23, RMJ21, Sch22b, YW20].  
**nonelectrostatic** [VL22]. **nonequilibrium** [MPP23]. **nonfullerene**  
 [TANC23]. **Noniterative** [HFPS20]. **Nonlinear** [BSR22, SNN<sup>+</sup>21].  
**nonlocal** [RMJ21, TV22, YW20]. **Nonredundant** [XZ20]. **Nonrigid**  
 [Bal20b]. **nonuniform** [YLZ<sup>+</sup>20]. **norbornadiene** [Dor20]. **norbornene**  
 [MCD22]. **norcarane** [MNH21]. **Normal** [San21]. **Normal-mode** [San21].  
**norovirus** [LSC<sup>+</sup>23]. **Novel**  
 [SEBE21, LHC<sup>+</sup>21, PPP21, RDK<sup>+</sup>22, SS20, VWP<sup>+</sup>22]. **ново**  
 [PMT<sup>+</sup>22, TIK21]. **NS5B** [MPuS<sup>+</sup>20]. **NSP15** [SLMA21]. **nuclear**  
 [IN23b, KE23b, LCC<sup>+</sup>21, LL21b, VCL20].  
**nuclear-magnetic-resonance-assisted** [LL21b]. **nucleation** [KEK23].  
**nucleobases** [CTBB20]. **nucleophilic** [CRT<sup>+</sup>21]. **nucleotide** [XZX<sup>+</sup>22].  
**Nudged** [MA23b, MA23a, ZLLL22]. **number** [MT20b]. **numbers**  
 [ASW20, SD21]. **numbers-based** [SD21]. **numerical**  
 [CX21b, DWZ22, GWN21, Pan23].

**O** [GJL21, KPTT21, LZW<sup>+</sup>23, TTK23, AWK<sup>+</sup>23, DK23, KPTT21, MC23,  
 MCP23, MBBU23, SWF<sup>+</sup>20, SWM<sup>+</sup>20b, SVTK<sup>+</sup>22, TYZ20]. **O-compounds**  
 [MCP23]. **O-H** [KPTT21]. **Obelin** [GOY20]. **obtain** [FNY21]. **obtained**  
 [UKBD23]. **OC** [HS23]. **occupation** [ASW20, Sch22a, SD21]. **occupied**  
 [KPHV23]. **OCOH** [dCVARN20]. **octamer** [Bal20b]. **octanol** [SHH<sup>+</sup>23b].  
**OCTMCCO** [LZW<sup>+</sup>23]. **O =** [ARR22b]. **off** [LK22]. **off-center** [LK22].  
**offs** [WKL22]. **oligonucleotides** [KZOV23]. **Omicron** [KLZ<sup>+</sup>23].  
**on-surface** [LHG<sup>+</sup>23]. **on-the-fly** [OSHT20, RBM<sup>+</sup>23]. **one**  
 [BBC<sup>+</sup>21a, WKG<sup>+</sup>23]. **one-electron** [BBC<sup>+</sup>21a]. **one-step** [WKG<sup>+</sup>23].  
**online** [WRVP22]. **onto** [AWK<sup>+</sup>23]. **OO** [SVTK<sup>+</sup>22]. **open**  
 [AAID22, FR21, HAC<sup>+</sup>23b, MNBG<sup>+</sup>21, PSGL21, RBM<sup>+</sup>23]. **open-source**  
 [AAID22, FR21, HAC<sup>+</sup>23b, MNBG<sup>+</sup>21, PSGL21, RBM<sup>+</sup>23]. **Opening**  
 [VDK<sup>+</sup>20]. **operators** [BBC<sup>+</sup>21a, CTPJH22]. **OPLS** [ZWY<sup>+</sup>22].  
**OPLS-AA** [ZWY<sup>+</sup>22]. **oppositely** [HPG20]. **optical**  
 [BA22, BSR22, JS21, JMV21, LRKD23, STB<sup>+</sup>20, Tou21]. **optically** [TIK21].  
**Optimal** [WZZ<sup>+</sup>20, YBS<sup>+</sup>20, SCvW22]. **Optimization**  
 [LPP20, MFS22, SSDL<sup>+</sup>23, AZKM22, CTPJH22, MLC<sup>+</sup>23, MZ21, MB21,  
 MT20b, NAAP21, PDGD22, PMT<sup>+</sup>22, SM20, SHH<sup>+</sup>23a, TV22].  
**optimizations** [GSD<sup>+</sup>22, MMK<sup>+</sup>20]. **Optimized** [GH22a]. **optimizing**

[RDB23]. **optoelectronic** [AQMM<sup>+</sup>23, ZGZ<sup>+</sup>20]. **orbit** [PHS<sup>+</sup>20, POPGS22]. **Orbital** [AD20, BBK20, KUNT20, LCC<sup>+</sup>21, SCKH21, AKN<sup>+</sup>20, ASW20, CB20, Fed22, GRBN21, HCS<sup>+</sup>20, KK23, KPHV23, NAN<sup>+</sup>23, NEG<sup>+</sup>20, PW20, Sch22b, SD21, TWT<sup>+</sup>22, TSH<sup>+</sup>23]. **orbital-based** [TWT<sup>+</sup>22]. **orbitals** [BTSB22, FV20, KL20, MH20]. **order** [CSGVF<sup>+</sup>20, DTA21, EVKL21, FKT21, FYIO23, GX20, HD21, QLV<sup>+</sup>22b, Sán20, YW20]. **Organic** [LPP20, AZKM22, FB20, GGK20, HRTSS<sup>+</sup>20, KGS<sup>+</sup>21, KS21, KPHV23, LPF<sup>+</sup>23, LMPT21, MAM21, MLP22, NI22, SC22, SZP<sup>+</sup>20, TANC23, TIK21, TSH<sup>+</sup>23, WP20, ZGZ<sup>+</sup>20]. **organic-inorganic** [KGS<sup>+</sup>21, SZP<sup>+</sup>20]. **organocatalysts** [FP22]. **organophosphorus** [TYZ20]. **orientation** [KPR23, RH21, SCC<sup>+</sup>22]. **oriented** [GZFSM21, NSRK21]. **Origin** [EK20b, MIK<sup>+</sup>23, PP23, RMS<sup>+</sup>23, DMTR22]. **Origins** [JFZ<sup>+</sup>20, TANC23]. **ortho** [VM23]. **ortho-nitrobenzaldehyde** [VM23]. **orthogonal** [CB20]. **oscillators** [BS23]. **Other** [FMFG20, TAC<sup>+</sup>23]. **overlap** [CTPJH22]. **Overlapping** [RTB23]. **Overreact** [SC23]. **Oversampling** [NNT<sup>+</sup>20]. **oxa** [NMMC21]. **oxa-Diels** [NMMC21]. **Oxidation** [CWZD20, KM22, LJW<sup>+</sup>23, MKB<sup>+</sup>21, PM21]. **oxidative** [IMT<sup>+</sup>21, KPDB22]. **oxide** [AMM22, MK22b, RMS<sup>+</sup>23, TYZ20]. **oxides** [RZS<sup>+</sup>23]. **Oxidized** [CWZD20]. **oxidozirconium** [CMD<sup>+</sup>22]. **oxindoles** [SKGG23]. **oxo** [MIP<sup>+</sup>22, MAM21]. **OxoMn** [MNH21]. **Oxygen** [GOY20, HL20, NAAP21]. **oxygen-oxygen** [HL20]. **oxynitride** [HM21].

**p** [ARA22, FBP<sup>+</sup>22, HYA<sup>+</sup>20, IW23, SSSA23, SHHH22]. **p-phenylenediamine** [ARA22]. **P-surface** [IW23]. **package** [AME<sup>+</sup>21, CKH23, HAC<sup>+</sup>23b, KZOV23, KYM20, LHH<sup>+</sup>21, MWK<sup>+</sup>20, SSDL<sup>+</sup>23, VWFR21, YWGY22]. **packet** [SWM<sup>+</sup>20b]. **Paddlewheel** [AD20]. **Pair** [SLR<sup>+</sup>20, GRBN21, HPG20, PW20, QLC<sup>+</sup>20, ZS22]. **pairs** [FP22, TTDT20]. **pairwise** [YBS<sup>+</sup>20]. **para** [SW21]. **para-substituted** [SW21]. **ParaCopasi** [YWGY22]. **parallel** [ABTM22, BBK<sup>+</sup>21, CP23, GVJ<sup>+</sup>22, JKK<sup>+</sup>21, JKS23, SSDL<sup>+</sup>23, WMZJ20, YWGY22]. **parallelization** [NN20, YLZ<sup>+</sup>20]. **parallelized** [AiIS<sup>+</sup>21]. **parameter** [POPGS22, RB22]. **parameterization** [OC23]. **Parameterizing** [KOD21]. **parameters** [DTA21, GH22a, KDLP21, LKM20, LBH<sup>+</sup>22, MH22, PNT<sup>+</sup>22]. **parametric** [PMT<sup>+</sup>22]. **parametrization** [GKO<sup>+</sup>22, KYM20]. **part** [MR21, MPR22, RLHG<sup>+</sup>23]. **partial** [LK22]. **particle** [CN21, WKD<sup>+</sup>21]. **particle-field** [WKD<sup>+</sup>21]. **particles** [LSC<sup>+</sup>23]. **partition** [AYO20, CSGVF<sup>+</sup>20, LC22, SHH<sup>+</sup>23b]. **Partitions** [TLD<sup>+</sup>22]. **Parzen** [AZKM22]. **Path** [SZLD20, Shi22, AKR21, GSD<sup>+</sup>22, RH21]. **paths** [ETT21b, MA23b, SDH23]. **pathway** [DSB23, HL20, PPRS22]. **pathways** [BBC20, CG20, DWSX20]. **patterns** [HS22, KLZ<sup>+</sup>23]. **Pb** [LXP<sup>+</sup>22]. **PbI** [XZW<sup>+</sup>21]. **PBSA** [SHH<sup>+</sup>23b, SHH<sup>+</sup>23a]. **PCM** [CC22]. **Pd** [ABZ20b, PTP23]. **Pd-PEPPSI** [ABZ20b]. **PDB** [RB22]. **PDB-to-parameter** [RB22]. **PdBe** [Tze21]. **PEACH** [ZK21]. **penicillin** [CD20]. **pentacoordinate** [FDK22]. **pentahalides** [PT21]. **Pep** [SKS21].

**PepPro** [XZ20]. **PEPPSI** [ABZ20b]. **peptidase** [CD20]. **Peptide** [XZ20, EIT<sup>+</sup>21, GG22, KZOV23, SKS21, SSS<sup>+</sup>20b, UAC<sup>+</sup>23].  
**peptide-based** [KZOV23]. **Peptide-Protein** [XZ20]. **per-** [MHA<sup>+</sup>23].  
**perfluorinated** [FDD<sup>+</sup>23]. **perfluoroalkyl** [MVV22]. **perform** [CKH23].  
**Performance** [BBK20, GSH23, NRH<sup>+</sup>20, PB20, BLB20, LKM20, MH22, MKK<sup>+</sup>22, OKI<sup>+</sup>21, dASRHB21, TTK23]. **performed** [MAM21].  
**Performing** [Zac20, FYIO23]. **period** [LB21, LB22]. **Periodic** [SDK20, HAC<sup>+</sup>23b, PKT21, PSMPB21, SZP<sup>+</sup>20, YAO20]. **permeability** [ZSD<sup>+</sup>20]. **permutation** [FYIO23]. **Permutationally** [OKK22]. **perovskite** [SZP<sup>+</sup>20, XZW<sup>+</sup>21]. **perovskites** [AQMM<sup>+</sup>23, ABAQ<sup>+</sup>23, KGS<sup>+</sup>21, dARW<sup>+</sup>23]. **peroxide** [CL23, DHN<sup>+</sup>21].  
**peroxides** [MC23, WKG<sup>+</sup>23]. **peroxy** [WKG<sup>+</sup>23]. **persistent** [BPDG21].  
**perspective** [AVM21, BBL<sup>+</sup>22, DF22, LKAT22, LT23, NI22, PPSP20, SWM<sup>+</sup>20b, SCC<sup>+</sup>22].  
**persulfate** [ARA22]. **Perturbation** [NNT<sup>+</sup>20, AAe20, FKT21, GX20, MH20, NTK21, OE20, Sán20, YBS<sup>+</sup>20].  
**perturbations** [PKT21]. **perturbed** [PDGD23]. **PFAS** [MPV22]. **Pfizer** [GLC<sup>+</sup>22]. **PH** [PT20, SSS<sup>+</sup>20a]. **pharma** [IRB<sup>+</sup>23]. **pharmacophore** [KDP<sup>+</sup>22, MLG<sup>+</sup>21b]. **pharmacophore-based** [MLG<sup>+</sup>21b]. **PharmRF** [KDP<sup>+</sup>22]. **Phase** [HFPS20, VFCG20, AZKM22, CM20a, DC22b, EK20c, IMT<sup>+</sup>21, LWF<sup>+</sup>22, OM23, SW21, WRBT21, YW20]. **phase-specific** [WRBT21]. **Phasepy** [CM20a]. **phenanthroline** [SGGG22].  
**phenomenological** [DWSX20]. **phenyl** [AS20, THLC<sup>+</sup>23].  
**phenylacetohydroxamic** [CMD<sup>+</sup>22]. **phenylenediamine** [ARA22, LDT<sup>+</sup>22]. **pheophytin** [Tou21]. **pHLIP** [FM21]. **Phonons** [DBE20]. **phosphate** [DPSG20, HUUO23, SGGG22]. **phosphoborane** [STB<sup>+</sup>20]. **phosphocholine** [ZK21]. **phosphodiester** [GP21].  
**phosphoglucose** [DPSG20]. **phosphorus** [ASL<sup>+</sup>20, HM21].  
**phosphorus-based** [ZS22]. **photo** [KFTB20b]. **photo-switchable** [KFTB20b]. **photoacidity** [GSH23]. **Photocatalytic** [BWS20].  
**photochemical** [CG20]. **Photochemistry** [FCPG20]. **photodynamic** [ASL<sup>+</sup>20, DART21, DMTR22]. **photoionization** [AAL21].  
**Photoisomerization** [YXGZ20]. **photooxidation** [KDKS21].  
**Photophysical** [DART21]. **photoproperties** [TANC23]. **Photoprotein** [GOY20]. **photoresponsive** [YLZ<sup>+</sup>22]. **photosensitizers** [ASL<sup>+</sup>20, DART21]. **photosensitizing** [HREvdK<sup>+</sup>20]. **photoswitches** [HPM<sup>+</sup>21]. **photovoltaic** [KGS<sup>+</sup>21]. **phthalocyanines** [DART21]. **Physical** [PFP<sup>+</sup>21, YJZ<sup>+</sup>22, BMT<sup>+</sup>21, Jab22b, RMS<sup>+</sup>23, TANC23]. **physico** [CSG<sup>+</sup>21]. **physico-chemical** [CSG<sup>+</sup>21]. **physicochemical** [KZP22].  
**physisorption** [RC22]. **PI** [AMM22]. **Picture** [QLW<sup>+</sup>22b, GCP22, JGGPN21]. **Picture-word** [QLW<sup>+</sup>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].

**platform** [BBB<sup>+</sup>23, CSG<sup>+</sup>21, PSGL21, ZK23]. **platform-independent** [CSG<sup>+</sup>21]. **platinum** [HBM<sup>+</sup>20, NAAP21]. **play** [FM21, KE23b]. **Plesset** [FKT21, CSGVF<sup>+</sup>20, Sán20]. **plugin** [EK20a]. **PMe** [PTP23]. **pockets** [XZX<sup>+</sup>22]. **Point** [MXM20, BSF20, CST23, MH22, PP23, PKT21, TTK23]. **points** [DTA21]. **Poisson** [CX21b, NSRK21, RCC21, SCvW22, WK21, XAD20]. **polarity** [DK23]. **polarizabilities** [LRKD23]. **polarizability** [OKK22]. **Polarizable** [HRT<sup>+</sup>20, LJ20, UB20, ALA<sup>+</sup>22, GP21, KLP<sup>+</sup>22, KYM20, KGD<sup>+</sup>21, LRqG<sup>+</sup>22, ODL20, WLWR22]. **Polarization** [Fed22, LB21, LB22, LLZ<sup>+</sup>23, MAM21, SKKK20, SSO<sup>+</sup>20]. **polarized** [NBE<sup>+</sup>23, PDGD23]. **Poltype** [WLWR22]. **poly** [LDT<sup>+</sup>22, MSA22a]. **polyacethylene** [BSR22]. **polyalcohol** [KSRB<sup>+</sup>21]. **polyatomic** [SSO<sup>+</sup>20]. **polyazaheterocycle** [MIP<sup>+</sup>22]. **polycyclic** [GAP21]. **polydiacetylene** [NLC23]. **polyenes** [FCB23]. **Polyethyleneimine** [BAC20, MT21, TPB22]. **Polyethylenimine** [MT20a, MT19]. **polyfluoroalkyl** [MHA<sup>+</sup>23]. **polymer** [WKD<sup>+</sup>21]. **polymeric** [AÁFJ21]. **polymerization** [ARA22, MLB<sup>+</sup>23, OSM20, XZZ<sup>+</sup>20]. **polymers** [LDT<sup>+</sup>22, MMK<sup>+</sup>20, VCL20]. **polymorphism** [CX23, RMS<sup>+</sup>23]. **polymorphs** [KGG21]. **polynomial** [OKK22]. **polyolefin** [KDKS21]. **polypeptoids** [RR22]. **polysulfides** [SC22]. **population** [LBH<sup>+</sup>22]. **porE** [TS21]. **porosities** [TS21]. **porous** [GGK20, SGT<sup>+</sup>20]. **porphyrin** [MNH21]. **porphyrinic** [KBHG23]. **Portably** [WMZJ20]. **Poses** [SZLD20]. **position** [FNY21, RH21]. **position-dependent** [FNY21]. **Positron** [SSO<sup>+</sup>20]. **possibilities** [LLKS23]. **possible** [ASL<sup>+</sup>20, DART21, SLMA21, WKG<sup>+</sup>23]. **posteriori** [BMT23, WFLZ23]. **potent** [BHR<sup>+</sup>21, ZOD<sup>+</sup>22]. **Potential** [KFTB20b, AS20, BBC<sup>+</sup>21a, EK20a, GFRNC21, GP21, HS23, HPM<sup>+</sup>21, KM22, KSRB<sup>+</sup>21, Kop22b, KGD<sup>+</sup>21, MSL<sup>+</sup>20, MK22b, OKI<sup>+</sup>21, PPRS22, RKC21, SDK20, Sts20, SSO<sup>+</sup>20, Tik23, WRVP22, XLW<sup>+</sup>22, YFH<sup>+</sup>21, ZZ23a]. **potential-energy** [MSL<sup>+</sup>20]. **potentials** [BSS<sup>+</sup>22, BBC<sup>+</sup>21a, GWN21, LT23, MLB<sup>+</sup>23, MAM<sup>+</sup>23, MLP22, RLHG<sup>+</sup>23, SM22b, SG20, TTK23, ZFRM20]. **ppdx** [COK22]. **precatalyst** [ABZ20b]. **precision** [XLW<sup>+</sup>22]. **preconditioning** [RH21]. **precursor** [BVC<sup>+</sup>23]. **precursors** [GM22]. **predefined** [BBSFA22]. **predict** [Ben22]. **predictability** [NGD22]. **Predicted** [CLS<sup>+</sup>20, LWF<sup>+</sup>22]. **Predicting** [APS20, BF22, HBT<sup>+</sup>20, QLW<sup>+</sup>22b, MPuS<sup>+</sup>20, MPV22, NTK21, PB20, SCZ<sup>+</sup>21]. **Prediction** [BUNO22b, CLS<sup>+</sup>20, DHD21, GOY20, LPP20, NMFI21, PWW20, SEZ20, SB20, SHHH22, SHH<sup>+</sup>23b, YFS20, ABZ20b, AAe20, AS23, DPY<sup>+</sup>22, Dor20, KZP22, KSRKS21, LRF<sup>+</sup>21, PWX<sup>+</sup>20, SHH<sup>+</sup>23a, TWT<sup>+</sup>22, UB20, XLW<sup>+</sup>22, YBS<sup>+</sup>20, YGG<sup>+</sup>23, ZHHS21, ZMH<sup>+</sup>21]. **predictions** [WCT<sup>+</sup>23]. **predictive** [FB20]. **prefer** [APS20]. **preference** [PFPD21]. **preferences** [DA22]. **Preliminary** [GP21, ZLLL22]. **preparation** [PBM21, QLC<sup>+</sup>20]. **prepare** [WKG<sup>+</sup>23]. **prepareforleap** [RB22]. **prepper** [KLP<sup>+</sup>22]. **Pressure** [HUUO23, SL20, EK20b, EK20c, GNL<sup>+</sup>22, KGG21]. **Pressure-assisted**

[HUUO23]. **pressure-induced** [EK20b, EK20c]. **primary** [ZWY<sup>+</sup>22]. **Principles** [DBE20, AWK<sup>+</sup>23, BRNB21, DLH<sup>+</sup>23, EK20b, EPT21, KDKS21, KPKS23, PM21]. **principles-based** [PM21]. **Probability** [TLD<sup>+</sup>22, RD23]. **probe** [NP23]. **Probing** [GH22a, WG20, Tou21]. **problem** [DWSX20, LBH<sup>+</sup>22]. **problems** [MA23b]. **Process** [WLZM20, BP22, KK23, PRH20, SS23, WG20, XZX<sup>+</sup>22, dCRM21]. **processes** [SSFS22b]. **Processing** [GCL<sup>+</sup>20, DWZ22]. **prodrug** [PRH20, PPSP20]. **Producing** [BP22]. **product** [WMZJ20]. **profile** [CSG<sup>+</sup>21]. **profiles** [HBM<sup>+</sup>20, SSS<sup>+</sup>20a]. **profiling** [SEBE21]. **program** [LKK<sup>+</sup>23, MNBG<sup>+</sup>21, PBM21, SWLC22, TSZ<sup>+</sup>21, WFBB22, XSP<sup>+</sup>23]. **Progress** [BGS<sup>+</sup>20]. **projection** [CTPJH22, VCL20]. **projections** [NEG<sup>+</sup>20]. **projector** [DGSB<sup>+</sup>20, NEG<sup>+</sup>20]. **projector-augmented-wave-based** [NEG<sup>+</sup>20]. **projector-based** [DGSB<sup>+</sup>20]. **prolapse** [GH22b]. **proline** [HB21]. **promenades** [MSL<sup>+</sup>20]. **Promising** [CP23]. **promoted** [OSM20]. **promotion** [MGCM21]. **propene** [LLS<sup>+</sup>22b]. **propensities** [DB23]. **propensity** [KPKS23]. **Properties** [DBE20, GOY20, HZG<sup>+</sup>20, SL20, SB20, ARR22a, ABAQ<sup>+</sup>23, AS20, BWS20, BA22, BSR22, BTSB22, CdSB<sup>+</sup>21, CM20a, CSG<sup>+</sup>21, CA22, DART21, DYGM21, HD21, IW23, JS21, JMV21, KPTT21, KBHG23, LRF<sup>+</sup>21, LWF<sup>+</sup>22, LRKD23, LXP<sup>+</sup>22, LDT<sup>+</sup>22, MMAZ<sup>+</sup>23, MCD22, NPGP23, PSM<sup>+</sup>20, PCI23, RMS<sup>+</sup>23, SBFSJMLU23, SGT<sup>+</sup>20, STB<sup>+</sup>20, VV20b, WSV20, WMJ<sup>+</sup>22]. **Property** [GZFSM21]. **Property-oriented** [GZFSM21]. **propylene** [AMM22]. **protease** [BVC<sup>+</sup>23, dSCCN21, PWX<sup>+</sup>20, PPP21, UAC<sup>+</sup>23, YC23]. **Protein** [BWM20, BSL20, CLS<sup>+</sup>20, HC21, LYKS23, MXM20, SZLD20, TWT<sup>+</sup>22, XZ20, ABTM22, AVM21, BK22, BPL<sup>+</sup>22, BBSFA22, BLB20, BAO<sup>+</sup>20, BF22, BVC<sup>+</sup>23, CDCT21, CH23, COK22, HTFY21, KCGK20, KR23, KGTL21, KSRKS21, KDP<sup>+</sup>22, KTM<sup>+</sup>23, LLS22a, LSP23, LL21b, LL22, MGB<sup>+</sup>22, MK22a, OC23, PDC23, QLW<sup>+</sup>22b, RDK<sup>+</sup>22, San21, SKL23, SY21, SEZ20, SLMA21, SNW22, WGKG20, YIO20]. **protein-glycosaminoglycan** [MGB<sup>+</sup>22]. **Protein-Ligand** [MXM20, LYKS23, TWT<sup>+</sup>22, KDP<sup>+</sup>22]. **Protein-Protein** [BSL20, COK22]. **protein-state** [BPL<sup>+</sup>22]. **Proteins** [HHL<sup>+</sup>20, LJ20, BPDG21, CCHS23, DB23, DO20, HB21, KCF<sup>+</sup>20, KOD21, LYKS23, LGC21, NYM22, POvG21, PPRS22, SSDL<sup>+</sup>23, TTH<sup>+</sup>21a, VWJ23]. **ProteinUnet** [KSRKS21]. **protic** [OM22]. **protocol** [ABNG22, Ben22, LCP21, MPP23, MPV22, VWP<sup>+</sup>22]. **Proton** [MFC20, AIV20, BBC20, DC22b, RCC<sup>+</sup>20, SW21]. **Protonated** [BAC20, MT21, ZHHS21]. **protons** [LL21b]. **protoporphyrin** [KPR23]. **prototyping** [KRSD<sup>+</sup>23]. **provide** [UB20]. **proximity** [WCD<sup>+</sup>23]. **proximity-enforced** [WCD<sup>+</sup>23]. **Prp** [RDK<sup>+</sup>22]. **Pseudodiagonalization** [SM20]. **Pseudodiagonalization-based** [SM20]. **pseudoknots** [YFH<sup>+</sup>21]. **Pseudomonas** [VDK<sup>+</sup>20]. **Pseudopotentials** [KGTL21]. **Pseudospectral** [CHVF21]. **Psi4** [EK20a]. **PSIXAS** [EK20a]. **Pt** [DZL<sup>+</sup>20, PTP23, PPSP20, SVDS21, SSM21]. **pucker** [KB22]. **pull**

[ARR22a, GPM21b, KdILC22]. **pulse** [LAM<sup>+</sup>23]. **pure** [BUNO22b, WMJ<sup>+</sup>22]. **purpose** [BMT<sup>+</sup>21, Mar21]. **purposes** [DF22, PFPD21]. **push** [ARR22a, GPM21b, KdILC22]. **push-pull** [ARR22a, GPM21b, KdILC22]. **putative** [CDCT21]. **puzzling** [XCJ20]. **PyCDFT** [MWK<sup>+</sup>20]. **PyFREC** [Kos22]. **PYK2** [SNW22]. **PyRad** [AME<sup>+</sup>21]. **pyranose** [KB22]. **pyrazine** [MH20]. **pyrazole** [BHR<sup>+</sup>21]. **PyRETIS** [RLR<sup>+</sup>20]. **pyridine** [PT21, YFS20]. **pyrido** [MIP<sup>+</sup>22]. **pyrimidin** [MIP<sup>+</sup>22]. **pyrimidin-3-yl** [MIP<sup>+</sup>22]. **pyrolysis** [KK22a]. **pyrrolylenones** [ARR22b]. **PySCF** [HAC<sup>+</sup>23b]. **Python** [CM20a, DMD<sup>+</sup>21, KRSD<sup>+</sup>23, LHH<sup>+</sup>21, MWK<sup>+</sup>20, PSGL21, VAP<sup>+</sup>21, WRBT21]. **Python-based** [LHH<sup>+</sup>21]. **PyUNIxMD** [LHH<sup>+</sup>21]. **PyVisA** [AKR21].

**Q** [SK20, ZDBZ20]. **Qball** [AME<sup>+</sup>21]. **QC** [KGD<sup>+</sup>21]. **QM** [Mar21, ABNG22, BBC20, GH22a, LRqG<sup>+</sup>22, Mar21, PWW20, PCI23, SSS<sup>+</sup>20a]. **QM/MM** [ABNG22, BBC20, GH22a, LRqG<sup>+</sup>22, Mar21, PCI23, SSS<sup>+</sup>20a]. **QM/QM** [PWW20]. **QMCube** [Mar21]. **QSAR** [BHR<sup>+</sup>21, DF22, SS20]. **QSAR/MD** [HKFT21]. **QSARINS** [CSG<sup>+</sup>21]. **QSARINS-Chem** [CSG<sup>+</sup>21]. **QTAIM** [AMF<sup>+</sup>20]. **quadrature** [IN23a]. **Quadruple** [Tze21, PTP23]. **Qualitatively** [Sts20]. **Quality** [RD23, AVM21, FB20, LB21, LB22, MK22a, SLB23]. **Quantification** [AWK<sup>+</sup>23]. **quantify** [LKK<sup>+</sup>23, Sch22b]. **quantifying** [IBL20]. **Quantitative** [AV20, BGS<sup>+</sup>20]. **quantity** [RD23]. **quantized** [VCRP23]. **Quantum** [AWID<sup>+</sup>20, IRB<sup>+</sup>23, OYO20, PAS<sup>+</sup>20, PHS<sup>+</sup>20, Pil20, SR23, AA20, BS23, BRNB21, BHR<sup>+</sup>21, BBK<sup>+</sup>21, CLTmd<sup>+</sup>23, CSGVF<sup>+</sup>20, CP23, FDK22, GPEK<sup>+</sup>20, GP21, HKS20, HUUO23, HBT<sup>+</sup>20, JCMHT22, JGGPN21, KRSD<sup>+</sup>23, KFLP21, KB22, LGM20, LGM22, LYX<sup>+</sup>22, MLC<sup>+</sup>23, OKI<sup>+</sup>21, OE20, PWX<sup>+</sup>20, PGP<sup>+</sup>21, RDB23, SPSH20, SSMP23, SIW21, SYS<sup>+</sup>21, SC23, SNN<sup>+</sup>21, Shi22, SCC<sup>+</sup>22, TPD21, TCS<sup>+</sup>21a, VWJ23, XSP<sup>+</sup>23]. **quantum-chemical** [BHR<sup>+</sup>21, SCC<sup>+</sup>22, VWJ23]. **quantum-classical** [HUUO23]. **quasi** [Cer22, NSKN21]. **quasi-degenerate** [NSKN21]. **quasi-harmonic** [Cer22]. **quaternary** [ODL20]. **quaterthiophene** [CBF<sup>+</sup>20]. **QuBiLS** [GJMPVR<sup>+</sup>20]. **QuBiLS-MIDAS** [GJMPVR<sup>+</sup>20]. **quest** [MMAZ<sup>+</sup>23]. **quick** [Vyb23]. **quinoline** [RLHG<sup>+</sup>23].

**R** [GGK20, LR20]. **R-C** [LR20]. **R61** [CD20]. **Rabenstein** [MDO<sup>+</sup>20]. **radial** [CBF<sup>+</sup>20]. **radical** [GNK<sup>+</sup>23, MP23, PFSC20, SKGG23]. **radical-mediated** [SKGG23]. **radicals** [WKG<sup>+</sup>23]. **radii** [SHH<sup>+</sup>23a]. **radiolysis** [AME<sup>+</sup>21]. **Raman** [CV22, GPEK<sup>+</sup>20, MH20, PGP<sup>+</sup>21]. **Random** [HFPS20, VFCG20, YW20]. **Range** [BBK20, AS21, CHVF21, GH22a, GAP21, HTFY21, HCS<sup>+</sup>20]. **ranking** [PNT<sup>+</sup>22]. **Raphson** [MT20b]. **Raphson/singular** [MT20b]. **rapid** [LLZ<sup>+</sup>23, MT20b]. **rare** [RLR<sup>+</sup>20, RD23]. **Ras** [MM20]. **Rashba** [dARW<sup>+</sup>23]. **rate** [dCVARN20]. **rates** [CGMRVBAI22]. **Rational**

[DSK21, SHP<sup>+23</sup>, ZZG<sup>+21</sup>, ZBH<sup>+23</sup>]. **ray** [EK20a, FB20]. **Rb** [SL20, AQMM<sup>+23</sup>, RNP20]. **RBD** [KLZ<sup>+23</sup>]. **RC**  $\equiv$  [WLZM20]. **RDFE** [MPP23]. **R**  $\equiv$  [WLZM20]. **Reaction** [QB20, SLR<sup>+20</sup>, AMM22, BBY<sup>+21</sup>, BBC20, BCN22, CG20, CS20, CD20, CRT<sup>+21</sup>, DWSX20, DPY<sup>+22</sup>, DLH<sup>+23</sup>, GSD<sup>+22</sup>, HL20, HREvdK<sup>+20</sup>, LLS<sup>+22b</sup>, LRqG<sup>+22</sup>, LBH<sup>+22</sup>, MNZGO<sup>+20</sup>, MIP<sup>+22</sup>, MNBG<sup>+21</sup>, MA23b, NAAP21, PRF20, PM21, SYS<sup>+21</sup>, SSS<sup>+20a</sup>, SKGG23, SSM21, SCZ<sup>+21</sup>, TYZ20, YGG<sup>+23</sup>, ZLLL22, ZS22]. **Reactions** [OOY20, SK20, ABZ20b, GCP22, LHG<sup>+23</sup>, MH22, MDO<sup>+20</sup>, MN20, PRF20, RCC<sup>+20</sup>, SYS<sup>+21</sup>, SC23, SMB<sup>+23</sup>, SSB<sup>+23</sup>, WKCP21, dCVARN20]. **Reactive** [TSH<sup>+23</sup>, BJ22, FVSS20, ZG21]. **Reactivities** [MML<sup>+23</sup>]. **Reactivity** [SHM<sup>+20</sup>, VAL20, CMD<sup>+22</sup>, GM22, KFLP21, LGJF22, LMPT21, MAI22, ZS22]. **reading** [VAP<sup>+21</sup>]. **reagents** [SCZ<sup>+21</sup>]. **Real** [MSS20, GCP22, HAC<sup>+23b</sup>, KdILC22]. **Real-time** [MSS20, HAC<sup>+23b</sup>]. **Realistic** [IN23b, ZWY<sup>+22</sup>]. **reality** [MSL<sup>+20</sup>]. **Realization** [SH23]. **Rearrangement** [PGP<sup>+23</sup>]. **reason** [RTB23]. **Reasoning** [QB20].

**Receptor** [BWM20, BRNB21, BHR<sup>+21</sup>, CSP20, TPZ<sup>+20</sup>, TZS<sup>+22</sup>, VWP<sup>+22</sup>, WGKG20]. **receptor-** [CSP20]. **receptor-flexible** [VWP<sup>+22</sup>]. **Receptor-Membrane** [BWM20]. **Receptors** [Min20]. **recognition** [BPL<sup>+22</sup>, BRNB21, DPSG20, KGD<sup>+21</sup>, SCCZ21, WCT<sup>+23</sup>]. **Recognizing** [HGF20]. **reconstruction** [ABTM22, PPV<sup>+21</sup>]. **reconstructions** [OAC23]. **Record** [HZG<sup>+20</sup>]. **Recovering** [RGGD21]. **recovery** [DK23]. **rectangular** [AYO20]. **recurrence** [Gao20, IN23a]. **recurrence-relation** [Gao20]. **recurrent** [TIK21]. **Redox** [RvWH23, MLB<sup>+23</sup>, RLHG<sup>+23</sup>, SM22b]. **Redox-active** [RvWH23]. **reductase** [CFOMCB<sup>+22</sup>]. **Reduction** [ABZ20b, AR20, NAAP21, PPSP20]. **reference** [BTSB22, KWYN23, VM23, WKL22]. **Refined** [KSRB<sup>+21</sup>]. **refinement** [NSRK21, RCC21]. **regime** [FCPG20]. **regio** [SMB<sup>+23</sup>]. **regio-** [SMB<sup>+23</sup>]. **region** [FKT21]. **Regioselective** [JFZ<sup>+20</sup>]. **Regioselectivity** [JFZ<sup>+20</sup>]. **regression** [BP22, OKK22, SS23]. **regularized** [SS23]. **regulating** [PPRS22, WSV20]. **regulator** [CDCT21]. **reinforcement** [JGK<sup>+22</sup>]. **related** [BPL<sup>+22</sup>, CdSB<sup>+21</sup>, MLB<sup>+23</sup>]. **relation** [Gao20]. **relationship** [HS22]. **relationships** [MML<sup>+23</sup>]. **relative** [MPP23, PWX<sup>+20</sup>]. **Relativistic** [GH22b, KWYN23, MCD22, RNP20, SDK20]. **relaxation** [GNK<sup>+23</sup>]. **release** [GGK20, Gie21, PRH20]. **relevant** [DF22, GKA<sup>+23b</sup>]. **Reliability** [ZWR22, Sch22b]. **Reliable** [PFSC20, AD23, CK22]. **REMD** [MGB<sup>+22</sup>]. **removal** [FNY21]. **renormalization** [BBK<sup>+21</sup>, TT20, XSP<sup>+23</sup>]. **repair** [CGMRVBAI22]. **Replacement** [ZXD20a, ZXD20b]. **replica** [FYIO23, JKS23, KN21, MGB<sup>+22</sup>, MZMK<sup>+21</sup>, RR22, SEZ20]. **replicas** [SDH23]. **repositioning** [SLMA21]. **Representation** [WZZ<sup>+20</sup>, BLB20, DF22, OKK22]. **Representations** [Bal20a, SBG20, CN21]. **repulsion** [KDLP21]. **repulsion-corrected** [KDLP21]. **repulsive** [MGB<sup>+22</sup>, MZMK<sup>+21</sup>, SEZ20]. **repurposed** [PPRS22]. **Repurposing** [EIT<sup>+21</sup>]. **residue** [BPL<sup>+22</sup>]. **residues** [MAP<sup>+20</sup>].

**resistance** [BF22]. **resolution** [LSP23]. **resolved** [AS21, ABNG22, CS23].  
**Resolving** [XCJ20]. **Resonance** [WG21, AV20, ARR22b, LL21b, NHFS21, Wan21a, Wan21b].  
**resonance-assisted** [AV20, ARR22b]. **resonances** [BBY<sup>+</sup>21]. **resource** [LGD<sup>+</sup>20]. **respect** [CC22]. **Response** [Wan21a, CC22, Tou21]. **responsive** [KCF<sup>+</sup>20]. **Restoring** [WKD<sup>+</sup>21]. **restrained** [QLC<sup>+</sup>20].  
**restrained-ensemble** [QLC<sup>+</sup>20]. **Restrains** [MXM20]. **Results** [BdLC21, Sts20]. **revealed** [LHG<sup>+</sup>23]. **revealing** [ARR22b]. **reveals** [BPDG21, HREvdK<sup>+</sup>20, JRS20, MAM21, ONA<sup>+</sup>20]. **Review** [ZFRM20].  
**revisited** [NSH23, PC23, SWF<sup>+</sup>20, TTT<sup>+</sup>21]. **Revisiting** [MMAZ<sup>+</sup>23, SCZ<sup>+</sup>21]. **RhB** [Tze21]. **rheology** [NP23]. **Rhodopsins** [HREvdK<sup>+</sup>20]. **riboswitches** [AAe20]. **ribozyme** [JRS20]. **rich** [JMV21, SCCZ21]. **Riemann** [MA23a]. **right** [SCZ<sup>+</sup>21]. **Rigid** [Min20, WCD<sup>+</sup>23]. **Ring** [LJ20, AG21, Jab22b, KB22]. **rings** [HS22, HS23].  
**RISM** [CKH23, YIO20]. **RL** [JGK<sup>+</sup>22]. **Rn** [APR21]. **RNA** [AAe20, KR23, SCCZ21, TM20, WCT<sup>+</sup>23, YFH<sup>+</sup>21]. **robust** [NMF121].  
**Role** [MKSS20, MAP<sup>+</sup>20, NAAP21, BVC<sup>+</sup>23, FM21, GCP22, KE23b, LKT21, MCD22, SGGG22, ZG21, ZOD<sup>+</sup>22]. **roles** [VV20b]. **rotamers** [FPF<sup>+</sup>21]. **rotating** [YrYqLhC23]. **rotation** [Kop22b]. **rotational** [PSMPB21]. **rotors** [YrYqLhC23]. **route** [SSM21]. **Roux** [IBL20].  
**rovibrational** [SR23]. **RS** [MGB<sup>+</sup>22, SHHH22, VAL20]. **RS-REMD** [MGB<sup>+</sup>22]. **Ru** [HSG21, ĆPP<sup>+</sup>22]. **rubber** [MML<sup>+</sup>23]. **RuBisCO** [DGSB<sup>+</sup>20, JMK<sup>+</sup>20]. **RuC** [Tze21]. **rule** [TLD<sup>+</sup>22, TTT<sup>+</sup>21]. **rung** [RMJ21]. **rung-3.5** [RMJ21]. **ruthenium** [KK23, YYS20]. **rutile** [VTdlM20].

**S** [DBE20, GCP22, Gie21, SLR<sup>+</sup>20, PWW20]. **SA** [Sts20]. **SA-2-CASSCF** [Sts20]. **saddle** [MH22]. **safe** [JRS20]. **salts** [JMV21]. **same** [Sán20].  
**same-spin** [Sán20]. **Sampling** [FMFG20, RD23, AKR21, FYIO23, GVJ<sup>+</sup>22, KN21, KSRB<sup>+</sup>21, LGC21, Ngo21, PPV<sup>+</sup>21, SBD<sup>+</sup>21, SSS<sup>+</sup>20a, STR20, WLSC23a, ZGZC20, ZKJ<sup>+</sup>23].  
**sandwich** [AS23, KBHG23]. **SARS** [EIT<sup>+</sup>21, KLZ<sup>+</sup>23, ONA<sup>+</sup>20, PDC23, PPP21, PPRS22, SLMA21, UAC<sup>+</sup>23, YC23]. **SARS-CoV-** [SLMA21].  
**SARS-COV-2** [ONA<sup>+</sup>20, EIT<sup>+</sup>21, KLZ<sup>+</sup>23, PDC23, PPP21, PPRS22, YC23]. **save** [POvG21]. **scalar** [RNP20]. **scale** [ARR22a, BGS<sup>+</sup>20, CJHW21, HREvdK<sup>+</sup>20, JKK<sup>+</sup>21, LSC<sup>+</sup>23, RDS<sup>+</sup>20, SY21, UAC<sup>+</sup>23]. **scaled** [Sán20].  
**scaling** [ASW20, CC22, MKK<sup>+</sup>22, MGB<sup>+</sup>22, MZMK<sup>+</sup>21, RR22, SEZ20, ZWY<sup>+</sup>22].  
**scattering** [CV22, DHD21, MH20]. **SCH** [SVTK<sup>+</sup>22]. **scheduling** [MLC<sup>+</sup>23]. **Scheme** [BSL20, GRN20, FCPG20, Gao20, LLZ<sup>+</sup>23, MT20b, RH21, STR20, VWJ23, ZZ23a]. **schemes** [DO20, HD21, MPP23]. **schiff** [ZRSST20]. **Schwarz** [IW23]. **Science** [PAF<sup>+</sup>20, PSG121]. **Scope** [TZS<sup>+</sup>22].  
**Scoring** [LAM<sup>+</sup>23, AMF<sup>+</sup>20, KDP<sup>+</sup>22]. **Scorpionates** [FNPD22].  
**scramblase** [KCF<sup>+</sup>20]. **screened** [YW20]. **screening** [AR20, CJHW21,

KDP<sup>+</sup>22, LCP21, MLG<sup>+</sup>21b, MPR22, NBE<sup>+</sup>23, UAC<sup>+</sup>23, WRVP22]. **Se**  
 [JS21, KPTT21, AQMM<sup>+</sup>23]. **Search** [BW22b, BAO<sup>+</sup>20, TIK21]. **Searching**  
 [DTA21, ZDBZ20]. **second**  
 [CC22, CSGVF<sup>+</sup>20, FKT21, GX20, Sán20, YW20]. **second-order**  
 [CSGVF<sup>+</sup>20, FKT21, GX20, Sán20, YW20]. **Secondary**  
 [AD20, AAe20, HC21, JRS20, KSRKS21]. **sections**  
 [ALA20, CV22, dBCdL20]. **selected** [CN21, KZOV23]. **selected-CI** [CN21].  
**selection** [BPL<sup>+</sup>22, SKL23]. **selective** [HRTSS<sup>+</sup>20, YLZ<sup>+</sup>22, ZOD<sup>+</sup>22].  
**selectivity** [FDD<sup>+</sup>23, KPKS23, MIK<sup>+</sup>23, NMMC21, SMB<sup>+</sup>23, SKGG23].  
**selenium** [ZGZ<sup>+</sup>20]. **selenium-containing** [ZGZ<sup>+</sup>20]. **selenolate**  
 [KPTT21]. **self**  
 [ASW20, BUNO22b, CV22, CQSG20, CTPJH22, MAP<sup>+</sup>20, PRH20, SKKK20].  
**self-assembly** [MAP<sup>+</sup>20, PRH20]. **self-consistent**  
 [CV22, CQSG20, CTPJH22, SKKK20]. **self-diffusion** [BUNO22b].  
**self-interaction** [ASW20]. **semi** [KB22, PWX<sup>+</sup>20, RLHG<sup>+</sup>23, TV22].  
**semi-empirical** [KB22, PWX<sup>+</sup>20, RLHG<sup>+</sup>23]. **semi-local** [TV22].  
**semiclassical** [FCB23]. **semiconducting** [CBF<sup>+</sup>20, KPHV23, LHC<sup>+</sup>21].  
**semiconductor** [LMPT21, WMJ<sup>+</sup>22, ZGZ<sup>+</sup>20]. **Semiempirical**  
 [GUCCR20, Gie21]. **Sensing** [HRTSS<sup>+</sup>20]. **Sensitivity** [BTSB22, LGM20].  
**sensitizers** [LCP21]. **sensor** [ZRSST20]. **sensors** [MK22b]. **Separated**  
 [BBK20]. **Separation** [NS22, WG20, YYZ<sup>+</sup>21]. **SEQCROW** [SIW21].  
**sequence** [KZOV23, KSRKS21, SBFSJMLU23]. **sequence-based**  
 [KSRKS21]. **sequential** [GGK20]. **series** [BHR<sup>+</sup>21, PWX<sup>+</sup>20]. **server**  
 [LGD<sup>+</sup>20, MPuS<sup>+</sup>20, FPMD23]. **serving** [TSH<sup>+</sup>23]. **Set**  
 [XZ20, YXGZ20, BK22, KS21, MCP23, SCKH21, TAC<sup>+</sup>23]. **sets**  
 [GZFSM21, GH22b, LB21, LB22, NSH23, RNP20, SLB23, SM22a]. **setup**  
 [CLTMd<sup>+</sup>23]. **seven** [KZJ22]. **seven-membered** [KZJ22]. **sextet** [TLD<sup>+</sup>22].  
**sH** [MJS<sup>+</sup>23]. **Sham** [BTSB22, EK20a, HCS<sup>+</sup>20, MB21]. **shape** [KTM<sup>+</sup>23].  
**SHARK** [Nee23]. **Shavitt** [SBG20]. **sheets** [SS23]. **shell**  
 [AME<sup>+</sup>21, Klo22, MB21, Sán20, PSMPB21]. **shift**  
 [FBP<sup>+</sup>22, TTDT20, UB20]. **shifts** [Ben22, MPV22, ZHHS21]. **shock**  
 [BAO<sup>+</sup>20, FVSS20]. **short** [HTFY21, SKKG22]. **short-range** [HTFY21]. **Si**  
 [GPM21b, WMJ<sup>+</sup>22, KPR23, VCRP23]. **side** [BSR22, ODL20, SSS<sup>+</sup>20b].  
**side-chain** [SSS<sup>+</sup>20b]. **signaling** [CDCT21]. **silaboryne** [DDSM23]. **silane**  
 [MML<sup>+</sup>23]. **silica** [MML<sup>+</sup>23]. **silica/rubber** [MML<sup>+</sup>23]. **silico**  
 [MAI22, SEBE21, SC23, PFPD21]. **Silicon**  
 [HZG<sup>+</sup>20, GPEK<sup>+</sup>20, PGP<sup>+</sup>21, ZXD20b, ZXD20a]. **siloxy** [LLS<sup>+</sup>22b]. **silver**  
 [FNP22]. **similar** [HGF20]. **similarity** [WRVP22]. **Simple**  
 [RH21, BW22a, BK22, Shi22, VWJ23]. **Simplex** [WSL<sup>+</sup>20]. **simplify**  
 [CTPJH22]. **simulate** [ABNG22, LRqG<sup>+</sup>22, TTH<sup>+</sup>21a, TMO<sup>+</sup>21].  
**simulated** [CS23]. **Simulating** [LA20, AME<sup>+</sup>21]. **Simulation**  
 [HZG<sup>+</sup>20, NNT<sup>+</sup>20, PAF<sup>+</sup>20, RR22, SL20, SNW22, BBC20, BP22, CDCT21,  
 CSP20, CBB<sup>+</sup>21, FNY21, GG22, HREvdK<sup>+</sup>20, HBM<sup>+</sup>20, KCGK20, KGS<sup>+</sup>22,  
 KLP<sup>+</sup>22, NLC23, NP23, ONA<sup>+</sup>20, PPP21, RKC21, SYS<sup>+</sup>21, SNN<sup>+</sup>21, SY21,

SWLC22, SCCZ21, UKBD23, VWFR21, YC23, YWGY22, ZK21].  
**simulation-based** [CDCT21]. **Simulations**  
 [SZLD20, Zac20, BUNO22b, DO20, EK20a, FCB23, FLT23, GGK20,  
 HUUO23, JKS23, LL21a, LKM20, LSC<sup>+</sup>23, LGC21, MPOC21, MSA22a,  
 Ngo21, NN20, NP23, PDC23, PBM21, PDL<sup>+</sup>21, PO<sub>v</sub>G21, PL22, PCI23,  
 QLC<sup>+</sup>20, RDK<sup>+</sup>22, RGGD21, SC23, SSDL<sup>+</sup>23, SKKK20, TTK23, TPB22,  
 Tik23, WCT<sup>+</sup>23, WGKG20, WFBB22, WKD<sup>+</sup>21, ZKJ<sup>+</sup>23]. **Simultaneous**  
 [GKO<sup>+</sup>22, BMT23, WFLZ23]. **single**  
 [AK20, BW22a, CBF<sup>+</sup>20, DLH<sup>+</sup>23, EVKL21, GSD<sup>+</sup>22, KSRKS21, VM23].  
**single-** [VM23]. **single-electron** [EVKL21]. **single-ended** [GSD<sup>+</sup>22].  
**single-molecule** [AK20]. **single-walled** [BW22a, CBF<sup>+</sup>20]. **single/dual**  
 [DLH<sup>+</sup>23]. **single/dual-atom** [DLH<sup>+</sup>23]. **Singlet**  
 [HFPS20, FCB23, LCP21, MdSJ<sup>+</sup>23, SCKH21]. **singular** [MT20b]. **Site**  
 [VGD<sup>+</sup>20, BBC20, CDCT21, CCHS23, DPSG20, KWYN23, KGD<sup>+</sup>21,  
 PLP<sup>+</sup>20, TZS<sup>+</sup>22, WKL22]. **site-specific** [CCHS23]. **sites**  
 [HGF20, LKM20, MAKZ23, YIO20]. **Si**  $\equiv$  [DDSM23]. **situ** [WKG<sup>+</sup>23].  
**situation** [FNPD22]. **situations** [THLC<sup>+</sup>23]. **six** [PTP23]. **six-electron**  
 [PTP23]. **sixth** [LB21]. **size**  
 [GH22b, HKSW20, JS21, KPR23, LBH<sup>+</sup>22, SSSA23, XAD20]. **size-modified**  
 [XAD20]. **Sized** [MFC20, BSS<sup>+</sup>22, ZDBZ20]. **slab** [VTdlM20]. **Slater**  
 [DWZ22, FV20, MFS22]. **Slater-type** [MFS22]. **sliced**  
 [GVJ<sup>+</sup>22, KN21, PPV<sup>+</sup>21]. **slip** [WKD<sup>+</sup>21]. **slip-springs** [WKD<sup>+</sup>21]. **Sm**  
 [ALA<sup>+</sup>22]. **Small** [LPP20, Mil21, GH22b, JS21, KYM20, LPF<sup>+</sup>23, MLP22,  
 NST<sup>+</sup>20, SKL23, TIK21, WLWR22, YIO20, ZK23, ZDBZ20].  
**small-molecule** [ZK23]. **small-sized** [ZDBZ20]. **Smoothed** [GJMPPB<sup>+</sup>20].  
**Sn** [LXP<sup>+</sup>22]. **sodium** [NSH23, SM22b]. **softness** [MAI22]. **Software**  
 [Kos22, Zac20, AG21, AME<sup>+</sup>21, CKH23, CJHW21, CSG<sup>+</sup>21, DMD<sup>+</sup>21,  
 GJMPPVR<sup>+</sup>20, HAC<sup>+</sup>23b, LHH<sup>+</sup>23, MLG<sup>+</sup>21b, RBM<sup>+</sup>23, SNN<sup>+</sup>21]. **solar**  
 [SZP<sup>+</sup>20, TANC23]. **Solid**  
 [TPD21, EG20, HM21, LB21, LB22, LZW<sup>+</sup>23, SLB23, UKBD23].  
**Solid-state** [TPD21, LB21, LB22, SLB23, UKBD23]. **solids** [CdSB<sup>+</sup>21].  
**solubility** [FLT23]. **Solute** [GRN20, JKS23, KN21, ZKJ<sup>+</sup>23]. **solution**  
 [KGS<sup>+</sup>22, KK23, KTM<sup>+</sup>23, MPOC21, RPD<sup>+</sup>20a, SH23]. **solutions**  
 [KSS21b, KSRB<sup>+</sup>21, SSS<sup>+</sup>20a]. **solvated** [LRKD23, MSA22b]. **Solvation**  
 [GRN20, LPF<sup>+</sup>23, MFC20, CKH23, CCHS23, GRBN21, GSH23, LML<sup>+</sup>23,  
 NML21, RPD<sup>+</sup>20a, SHH<sup>+</sup>23a, VL22, VV21, Vyb23, WKL22]. **solve** [MA23b].  
**Solvent** [BBK20, FMFG20, GCL<sup>+</sup>20, KWYN23, SLR<sup>+</sup>20, Sts20, CDCT21,  
 DK23, KK23, KPHV23, LML<sup>+</sup>23, MGB<sup>+</sup>22, PT21, SPSH20, SHHH22,  
 VCL20, WLSC23a, XAD20]. **solvent-accessible** [VCL20]. **solvents**  
 [OM22, RPD<sup>+</sup>20a, VV21]. **solver** [NSRK21, WK21]. **solving** [MB21]. **Some**  
 [QB20, MAI22]. **sorbitol** [KSS21b]. **source**  
 [AAID22, FR21, HAC<sup>+</sup>23b, MNBG<sup>+</sup>21, PSGL21, RBM<sup>+</sup>23]. **sp**  
 [AKN<sup>+</sup>20, PPP21]. **space**  
 [BAO<sup>+</sup>20, GCP22, HL20, KZOV23, MPR22, RSHG23, SBD<sup>+</sup>21, TZS<sup>+</sup>22].

**Sparse** [BPL<sup>+</sup>22]. **speciation** [LGD<sup>+</sup>20]. **species** [XAD20]. **specific** [CCHS23, WRBT21, ZKJ<sup>+</sup>23]. **Spectra** [CWZD20, CS23, EK20a, GPEK<sup>+</sup>20, KGS<sup>+</sup>22, LWLC21, PGP<sup>+</sup>21, SNN<sup>+</sup>21, TMO<sup>+</sup>21]. **spectral** [LDT<sup>+</sup>22]. **spectroscopic** [LZW<sup>+</sup>23]. **Spectroscopy** [BLP20, CMD<sup>+</sup>22, FB20, MPOC21, Sai23]. **spectrum** [AS21]. **speed** [GWN21, WFBB22]. **Spherical** [GJMPB<sup>+</sup>20]. **SPIDER3** [KSRKS21]. **SPIDER3-single** [KSRKS21]. **spike** [Jab22b, ONA<sup>+</sup>20, PDC23]. **spike-ring** [Jab22b]. **Spin** [IYI<sup>+</sup>20, SWF<sup>+</sup>20, SWM<sup>+</sup>20b, TPD21, GNK<sup>+</sup>23, HYA<sup>+</sup>20, KE23b, KKAK23, NBE<sup>+</sup>23, PDGD23, PHS<sup>+</sup>20, POPGS22, QLC<sup>+</sup>20, Sán20, VV20b, XCJ20]. **spin-coupled** [XCJ20]. **Spin-flip** [IYI<sup>+</sup>20, KKAK23]. **Spin-inversion** [SWF<sup>+</sup>20, SWM<sup>+</sup>20b]. **Spin-liquids** [TPD21]. **spin-orbit** [PHS<sup>+</sup>20, POPGS22]. **spin-pair** [QLC<sup>+</sup>20]. **spin-polarized** [NBE<sup>+</sup>23]. **spiropyran** [DK23]. **splicing** [SCCZ21]. **splitting** [OSHT20, YYS20, dARW<sup>+</sup>23]. **splittings** [SRB21]. **SPOT** [CLS<sup>+</sup>20]. **SPOT-Fold** [CLS<sup>+</sup>20]. **springs** [WKD<sup>+</sup>21]. **stabilities** [WKCP21]. **Stability** [GKA<sup>+</sup>23b, STB<sup>+</sup>20, VAL20, APR21, BK22, BPDG21, CCHS23, DDSM23, GM22, LML<sup>+</sup>23, MVV22, MdSJ<sup>+</sup>23, MJS<sup>+</sup>23, MIP<sup>+</sup>21, NLC23, PDC23, PB20, PP23, VTdlM20]. **Stabilization** [BD22, GPM21b, FM21, PFSC20]. **stabilized** [KW22, PLZT23, WCD<sup>+</sup>23]. **stabilizing** [DSB23]. **stacking** [XLW<sup>+</sup>22]. **Standalone** [KYM20, CSG<sup>+</sup>21]. **standard** [TZS<sup>+</sup>22]. **stannites** [MZ21]. **stannylenes** [BKM21]. **stars** [GSJ<sup>+</sup>23]. **State** [BWM20, BSF20, AIV20, BPL<sup>+</sup>22, CH23, FYIO23, HD21, HPM<sup>+</sup>21, KL20, KBHG23, Kop22b, LB21, LB22, LHH<sup>+</sup>21, OSHT20, RSHG23, RLHG<sup>+</sup>23, SLB23, Sts20, TPD21, Tou21, UKBD23, WD20, WMZJ20, ZRSST20, dCVARN20]. **State-of-the-art** [BSF20]. **states** [BMT23, BW22b, CG20, CPG21, EVKL21, FCB23, FB21, Gie21, HYA<sup>+</sup>20, IK21, JCMHT22, Kop22a, LJW<sup>+</sup>23, MdSJ<sup>+</sup>23, NBE<sup>+</sup>23, OMC<sup>+</sup>20, RDS<sup>+</sup>20, SDH23, SBB<sup>+</sup>22, VM23, WFLZ23]. **static** [EVKL21]. **Statistical** [AAe20, DC22b, UKBD23]. **steels** [ZFRM20]. **steered** [MK22a]. **step** [FR21, POvG21, WKG<sup>+</sup>23]. **step-length** [FR21]. **stepping** [MKK<sup>+</sup>22]. **stepping-based** [MKK<sup>+</sup>22]. **steps** [DGSB<sup>+</sup>20]. **stepwise** [KZJ22]. **stereo** [SMB<sup>+</sup>23]. **stereographic** [VCL20]. **Stereoselectivity** [WLZM20]. **Steric** [VDK<sup>+</sup>20, GCP22]. **stiffness** [MA23b]. **stochastic** [SSFS22b]. **stone** [CTBB20]. **stone-wales** [CTBB20]. **storage** [SKKG22, SSYB<sup>+</sup>20, WG20]. **Strain** [SLR<sup>+</sup>20, MGC21]. **strains** [LSC<sup>+</sup>23]. **Strategies** [PDGD22, PFPD21, SBB<sup>+</sup>22]. **strategy** [HB21]. **streamline** [PBM21]. **strength** [CVGVN<sup>+</sup>20, FDD<sup>+</sup>23, MVP<sup>+</sup>20, NTK21]. **Streptomyces** [CD20]. **stretching** [GAP21]. **strong** [FCPG20]. **strontium** [KGG21]. **Structural** [ABAQ<sup>+</sup>23, CM20b, MdSJ<sup>+</sup>23, PSM<sup>+</sup>20, SL20, WMJ<sup>+</sup>22, AVM21, FPMD23, ONA<sup>+</sup>20, QLW<sup>+</sup>22b, SH23, XZW<sup>+</sup>21, ZOD<sup>+</sup>22]. **Structure** [CLS<sup>+</sup>20, GLC<sup>+</sup>22, GG22, MJS<sup>+</sup>23, MIP<sup>+</sup>21, NLC23, WCD<sup>+</sup>23, XZ20, AAe20, ABTM22, AYO20, BLB20, DGSB<sup>+</sup>20, GH22a, GSD<sup>+</sup>22, GAG20, HC21, HSG21, HGF20, KWYN23, KDKS21, KPDB22, KDP<sup>+</sup>22, LSP23, LL21b,

MNH21, MZ21, MPV22, MK22a, NUK21, NHFS21, PDGD22, PP23, RKC21, RDK<sup>+</sup>22, RvWH23, SM22b, VTdlM20, VM23, WS21, XZW<sup>+</sup>21, ZWY<sup>+</sup>22]. **structure-** [GH22a]. **structure-based** [GLC<sup>+</sup>22, KDP<sup>+</sup>22, LSP23, RKC21]. **Structures** [CWZD20, HZG<sup>+</sup>20, LWF<sup>+</sup>22, ZBH<sup>+</sup>23, AAID22, AZKM22, DC22a, DTA21, DYGM21, KS21, KZP22, KGTL21, KSRKS21, LSP23, LXP<sup>+</sup>22, LL22, MH22, NSKN21, POPGS22, SAZ<sup>+</sup>23, TT20, WHJM23, YIO20, ZDBZ20, ZWR22]. **studied** [LL21a, SY21, WS21]. **Studies** [CWZD20, ARA22, CFOMCB<sup>+</sup>22, CX21b, CMD<sup>+</sup>22, DA22, FPMD23, GM22, HKS20, LGJF22, MSE<sup>+</sup>21, MSA22a, NLC23, RKC21, RR22, ZFRM20]. **Study** [JFZ<sup>+</sup>20, ARR22b, APS20, AMM22, ALA<sup>+</sup>22, BW22a, BA22, BBC20, BD22, CS20, CL23, CTBB20, CRT<sup>+</sup>21, DZL<sup>+</sup>20, DK23, DLH<sup>+</sup>23, DSK21, FDK22, HS22, HM21, HTFY21, HSG21, HCY<sup>+</sup>22, JC20, JMV21, KZJ22, KR23, KM22, KBHG23, KSRB<sup>+</sup>21, KEK23, KPKS23, LEP<sup>+</sup>21, LC22, LJW<sup>+</sup>23, MNH21, MNZGO<sup>+</sup>20, MLP22, MAP<sup>+</sup>20, NAAP21, NAN<sup>+</sup>23, NPGP23, OE20, OSM20, PRH20, Pan23, PDGD23, PM21, RPD<sup>+</sup>20a, RDS<sup>+</sup>20, SEBE21, dASRHB21, SVDS21, SSS<sup>+</sup>20a, SI22, SC22, TANC23, TMO<sup>+</sup>21, TLS23, TPZ<sup>+</sup>20, VTdlM20, WG20, WRBT21, WKG<sup>+</sup>23, YYS20, ZDBZ20, ZMH<sup>+</sup>21, ZG21]. **studying** [RDB23]. **style** [Tik23]. **styrene** [ZZG<sup>+</sup>21]. **sub** [NAAP21]. **subject** [LAM<sup>+</sup>23]. **subnanoclusters** [FBM<sup>+</sup>23]. **suboxide** [LZW<sup>+</sup>23]. **substances** [MHA<sup>+</sup>23, MVV22]. **substituent** [JK21, LGM20, LGM22, MAM21]. **Substituted** [NRH<sup>+</sup>20, ASL<sup>+</sup>20, BSR22, MNZGO<sup>+</sup>20, NMMC21, SW21, SMB<sup>+</sup>23]. **substitution** [ĆPP<sup>+</sup>22, HREvdK<sup>+</sup>20, JC20]. **Substitutional** [GPEK<sup>+</sup>20]. **substrates** [KCF<sup>+</sup>20]. **sugar** [SGGG22]. **suitable** [SHH<sup>+</sup>23a]. **suite** [Mar21]. **sulfide** [MSE<sup>+</sup>21]. **sulfuric** [KEK23]. **summation** [Pan23, WKL22, YLZ<sup>+</sup>20]. **superacids** [Brz23]. **Superalkalis** [Mil21]. **superatom** [YMSS23]. **supercomputer** [JKS23]. **superconductors** [TPD21]. **Superfamily** [MM20]. **superhalogens** [Mil21]. **superphane** [Jab22a]. **Superposition** [Wan21a, Wan21b, WG21]. **supersalts** [Mil21]. **superstructures** [TPD21]. **supported** [BWS20, DZL<sup>+</sup>20]. **supramolecular** [GBM20]. **Surface** [GCL<sup>+</sup>20, MH20, PAF<sup>+</sup>20, YXGZ20, FCPG20, IW23, LHG<sup>+</sup>23, MSE<sup>+</sup>21, OKI<sup>+</sup>21, PM21, SZP<sup>+</sup>20, SSM21, TV22, VCL20, WK21, XLW<sup>+</sup>22]. **Surface-enhanced** [MH20]. **surfaces** [AWK<sup>+</sup>23, DA22, HPM<sup>+</sup>21, LMPT21, MN20, MSL<sup>+</sup>20, OKK22, RDB23, Sts20, VCL20]. **surrounding** [Sch22a]. **SuSMoST** [PAF<sup>+</sup>20]. **swarms** [LA20]. **switchable** [KFTB20b]. **symmetry** [BPDG21, NTK21, NVBG23, OE20, PSMPB21, SM22b]. **symmetry-adapted** [NTK21, OE20]. **symmetry-decomposed** [NVBG23]. **synergistic** [PRH20]. **Synthesis** [MSE<sup>+</sup>21, KZJ22, SEBE21]. **System** [HHL<sup>+</sup>20, NAN<sup>+</sup>23, DGM22, Nee23]. **Systematic** [KUNT20, STR20, DSK21, TS21]. **Systems** [LR20, AAID22, EVKL21, GNK<sup>+</sup>23, HAC<sup>+</sup>23b, JKK<sup>+</sup>21, JKS23, LC22,

NLC23, PKT21, SIW21, UB20, WG20, YAO20].

**T** [CS20, CK22, CSWW20, Dor20, KG23, MLB+23, MEKH22, PRF20, SI22, 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]. **targets** [BF22]. **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]. **Teller** [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]. **terms** [GKO+22, MR21]. **test** [SHH+23b, SHH+23a]. **testing** [KG23, NGD22]. **tetra** [dSCCN21]. **tetra-coordinate** [dSCCN21]. **tetracoordinate** [DC22a]. **tetrafluoride** [Brz22]. **tetrahedral** [BA22]. **tetrahydro** [MSE+21]. **tetrahydro-** [MSE+21]. **tetrahydrodibenzazosines** [SS20]. **tetrakis** [MVP+20]. **tetranuclear** [KKAK23]. **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** [DA22, JMK+20, LGJF22, MML+23, VTdlM20, AQMM+23, BD22, BBL+22, HRTSS+20, HSG21, KDKS21, KK22a, MNZGO+20, NMFI21, OSM20, PRH20, TSH+23, ZS22]. **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, DZL+20, DC22b, DOT22, FB20, FKT21, GRBN21, GD23, GX20, HM21, HCS+20, JK21, KZJ21, KWYN23, KS21, KdlLC22, LGM20, LGM22, LYX+22, MWK+20, MNH21, MLB+23, MIP+22, MR21, MPR22, MFS22, MKB+21, MGCM21, MH20, MSS20, NHFS21, NTK21, NEG+20, OE20, OMC+20, RGGD21, SDK20, SWF+20, Sán20, dASRHB21, SC22, SMB+23, SSBYB+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]. **Thermal** [KTM+23, GGK20, LGJF22]. **thermally** [LYX+22]. **Thermochemical** [WKCP21, SSBYB+20]. **Thermochemistry** [MHA+23, DKB23, OM23, RMJ21]. **Thermodynamic** [DBE20, SZLD20, CCHS23, KCGK20, MAM+23]. **Thermodynamics** [SK20]. **thermoelectric** [AQMM+23, ABAQ+23]. **ThermoML** [RTB+22]. **thermophilic** [NYM22]. **Thermostabilization** [NYM22]. **ThetaPhi**

[TPD21]. **Thioflavin** [Sts20]. **thioformaldehyde** [SVTK<sup>+</sup>22]. **thioguanine** [NST<sup>+</sup>20]. **Thiols** [AWID<sup>+</sup>20]. **thione** [KGD<sup>+</sup>21, NST<sup>+</sup>20]. **thione-containing** [NST<sup>+</sup>20]. **thiophenols** [CGMRVBAI22]. **third** [GKO<sup>+</sup>22]. **third-neighbor** [GKO<sup>+</sup>22]. **those** [LML<sup>+</sup>23]. **Three** [PLP<sup>+</sup>20, LLZ<sup>+</sup>23, LSC<sup>+</sup>23, MP23, NYM22, YAO20]. **three-body** [LLZ<sup>+</sup>23]. **three-dimensional** [YAO20]. **three-helix** [NYM22]. **Three-site** [PLP<sup>+</sup>20]. **throughput** [MZ21, NBE<sup>+</sup>23]. **thymine** [SSS<sup>+</sup>20a]. **Ti** [AQMM<sup>+</sup>23]. **tight** [GH22a, IYI<sup>+</sup>20, MCP23, NBE<sup>+</sup>23, NN20, Pil20, RLHG<sup>+</sup>23, WKCP21]. **tight-binding** [IYI<sup>+</sup>20, NBE<sup>+</sup>23, NN20, RLHG<sup>+</sup>23]. **Time** [BA22, YXGZ20, ABNG22, CPG21, FB20, HAC<sup>+</sup>23b, IYI<sup>+</sup>20, KSRB<sup>+</sup>21, KdILC22, LSC<sup>+</sup>23, MKK<sup>+</sup>22, MFS22, MSS20, OMC<sup>+</sup>20, POvG21, TANC23]. **Time-Dependent** [YXGZ20, BA22, CPG21, FB20, IYI<sup>+</sup>20, MFS22, MSS20, OMC<sup>+</sup>20, TANC23]. **time-invariant** [KSRB<sup>+</sup>21]. **time-resolved** [ABNG22]. **timescale** [DWSX20]. **tiny** [ZWY<sup>+</sup>22]. **TiO** [VTdlM20]. **TITAN** [SHM<sup>+</sup>20]. **titanate** [KGG21]. **titania** [BWS20]. **titanium** [CMD<sup>+</sup>22]. **TI** [ABAQ<sup>+</sup>23, Sai23]. **TM** [LXP<sup>+</sup>22, LZW<sup>+</sup>23, LXP<sup>+</sup>22]. **TM-** [LZW<sup>+</sup>23]. **TMEM16** [KCF<sup>+</sup>20]. **Tool** [dSBFdAJ20, AAID22, ARR22b, FPMD23, GLC<sup>+</sup>22, LKM20, RB22, WRVP22, ZK23, ZGZC20]. **Toolkit** [PAF<sup>+</sup>20, AAFJ21, CLTMd<sup>+</sup>23, MPP23]. **Topological** [EK20c, AA20, EPT21, HBT<sup>+</sup>20]. **topology** [CP23, KFLP21, MPP23, MVP<sup>+</sup>20, PHS<sup>+</sup>20, Pil20]. **torsional** [GKO<sup>+</sup>22]. **toughness** [MMAZ<sup>+</sup>23]. **toxicity** [CSG<sup>+</sup>21, SEBE21]. **tracking** [BBB<sup>+</sup>23]. **trajectories** [AKR21, LA20]. **Trajectory** [OSHT20, YXGZ20, FCPG20, SWLC22, ZGZC20]. **transamination** [BBC20]. **transfer** [AIV20, BBC20, BBC<sup>+</sup>21a, BOPJ<sup>+</sup>21a, CPG21, IK21, KCGK20, KPR23, Kos22, OMC<sup>+</sup>20, RCC<sup>+</sup>20, SSYB<sup>+</sup>20, dCRM21]. **Transferability** [LGM22]. **transferable** [VL22]. **transform** [YLZ<sup>+</sup>20]. **transformation** [BLB20]. **transient** [ABNG22, BBL<sup>+</sup>22]. **Transition** [PWW20, AR20, BW22b, CH23, EK20a, EK20b, KL20, NBE<sup>+</sup>23, PDC23, PTP23, PDGD23, PSM<sup>+</sup>20, RSHG23, SDH23, SBB<sup>+</sup>22, VV20b, dCVARN20]. **Transition-Metal** [PWW20]. **transition-potential** [EK20a]. **transitions** [EK20c, HSG21]. **Transmembrane** [MKSS20, SSS<sup>+</sup>20b]. **Transport** [HHL<sup>+</sup>20, YC20, LEP<sup>+</sup>21, WSV20, XZW<sup>+</sup>21, ZGZ<sup>+</sup>20]. **trapping** [ZS22]. **treat** [SSDL<sup>+</sup>23]. **treatment** [Cer22, SLMA21]. **Tree** [AZKM22, AYO20, CN21, TIK21]. **treecode** [WKL22]. **trends** [SDK20]. **tri** [dSCCN21]. **tri-** [dSCCN21]. **Triacylglyceride** [CST23]. **triangulation** [WK21]. **triazole** [KGD<sup>+</sup>21]. **triazolotetrazine** [KZP22]. **Trichoderma** [HYA<sup>+</sup>20]. **tricoordinated** [THLC<sup>+</sup>23]. **triclesyl** [HUUO23]. **trifluoro** [SMB<sup>+</sup>23]. **trimeric** [PDC23]. **trimethylphosphine** [CS20]. **trioxides** [KZP22]. **tripeptide** [OAC23]. **tripeptides** [OAC23]. **triphosphate** [XZX<sup>+</sup>22]. **triple** [DTA21, LB21, LB22, SLB23, ZMH<sup>+</sup>21]. **triple-zeta** [LB21, LB22, SLB23]. **Triplet** [HFPS20, MdSJ<sup>+</sup>23]. **tris** [AS20, MCD22]. **tropolone** [OSHT20]. **truncated** [GJMPVR<sup>+</sup>20]. **Truncation** [GJMPB<sup>+</sup>20, NAN<sup>+</sup>23]. **tryptophane** [CGMRVBAI22]. **tuberculosis**

[RKC21, RDK<sup>+</sup>22]. **tumors** [CM20b]. **Tuning** [BKM21, BBK20, Cer22, MP23, ARR22a]. **tunneling** [OSHT20, SRB21]. **TUPÁ** [PL22]. **Two** [LHC<sup>+</sup>21, YrYqLhC23, BPDG21, FCB23, HYA<sup>+</sup>20, IN23a, KGS<sup>+</sup>21, KL20, PTP23, STB<sup>+</sup>20, VWJ23, Wan23, YAO20]. **two-body** [VWJ23]. **two-component** [KL20]. **two-dimensional** [STB<sup>+</sup>20]. **two-electron** [IN23a, PTP23]. **Two-layer** [YrYqLhC23]. **type** [ABZ20b, BVC<sup>+</sup>23, FV20, LL21a, LLKS23, MFS22, WKCP21, KUNT20]. **Type-1** [KUNT20].

**U** [SB20]. **ubiquitous** [PRF20]. **UG** [SCCZ21]. **UG-rich** [SCCZ21]. **UiO** [FP23]. **UiO-66** [FP23]. **Ullmann** [LHG<sup>+</sup>23]. **ultra** [SKKG22]. **ultra-short** [SKKG22]. **ultrafast** [BBL<sup>+</sup>22, LAM<sup>+</sup>23]. **ultrashort** [Jab22b]. **umbrella** [Ngo21, SSS<sup>+</sup>20a]. **Uncertainty** [HM21]. **unconstrained** [CRT<sup>+</sup>21]. **Uncovering** [GM22, TLD<sup>+</sup>22]. **underlying** [ONA<sup>+</sup>20, WFBB22]. **Understanding** [KZJ21, MGCM21, NVBG23, SMB<sup>+</sup>23, CX23]. **unique** [DYG21, KLZ<sup>+</sup>23]. **Unitary** [SBG20]. **Units** [AD20, GCL<sup>+</sup>20, DWZ22]. **universal** [LGM20, LGM22]. **Unlocking** [GUCCR20]. **Unprecedented** [JFZ<sup>+</sup>20]. **Unraveling** [BRNB21]. **UNRES** [SSDL<sup>+</sup>23]. **unusual** [LML<sup>+</sup>23]. **Unveiling** [IMT<sup>+</sup>21]. **updated** [MT20b]. **upon** [EK20c, YOCMA23]. **uranyl** [PB20]. **use** [BBB<sup>+</sup>23, CK22, COK22, POG21]. **useful** [ZGZC20]. **user** [SKS21, ZK23]. **user-friendly** [SKS21, ZK23]. **Using** [CTPJH22, GCL<sup>+</sup>20, KUNT20, LJ20, MK22a, VAL20, WZZ<sup>+</sup>20, AV20, BS23, BHR<sup>+</sup>21, BSL20, BSF20, BF22, CV22, CQSG20, CST23, DHD21, DGSB<sup>+</sup>20, GNK<sup>+</sup>23, HUUO23, HPM<sup>+</sup>21, IN23a, JGGPN21, KLP<sup>+</sup>22, KSRB<sup>+</sup>21, KB22, KdlLC22, LA20, LRF<sup>+</sup>21, LGC21, LWLC21, LDT<sup>+</sup>22, MPP23, MN20, MIP<sup>+</sup>22, MEKH22, MA23a, MSS20, NS22, OC23, PAS<sup>+</sup>20, PWX<sup>+</sup>20, PFPD21, QLW<sup>+</sup>22b, RR22, SW21, SK23, SEZ20, SSYB<sup>+</sup>20, SCCZ21, SHH<sup>+</sup>23b, TIK21, TLD<sup>+</sup>22, Tou21, WKCP21, WMZJ20, WKG<sup>+</sup>23]. **USPEX** [VWFR21]. **utilized** [GM22]. **utilizing** [HD21]. **UV** [CWZD20, LWLC21, TMO<sup>+</sup>21]. **UV-Vis** [CWZD20, LWLC21, TMO<sup>+</sup>21].

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- [Ano21d] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(4):205–209, February 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano21g] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(7):465–469, March 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- Anonymous:2022:IIg**
- [Ano22g] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(7):435–439, March 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano22h] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(8):499–503, March 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano22k] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(11):741–745, April 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano22m] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(13):889–893, May 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano22p] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(16):1063–1067, June 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano22q] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(17):1135–1139, June 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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