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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]. 4*H* [MSE<sup>+</sup>21]. 5 [AS20, JMV21, SDK20, VTdlM20]. 7 [MdSJ<sup>+</sup>23]. 8 [Bal20b]. [3 + 2] [BAM<sup>+</sup>24, SMB<sup>+</sup>23]. + [APR21, CWZD20, GJL21, KM24, LR20, LEP<sup>+</sup>21, MAM<sup>+</sup>23, OM22, WSV20, YMSS23]. - [Tze21, WSV20, WMJ<sup>+</sup>22]. <sup>1</sup> [ZHHS21]. <sup>13</sup> [KWX23, MCD22, ZHHS21]. <sup>19</sup> [Ben22, MPV22]. <sup>2</sup> [AKN<sup>+</sup>20]. <sup>2+</sup> [ALA<sup>+</sup>22, HSG21, IK21, JRS20, MAKZ23, SPSH20, ZRSST20]. <sup>205</sup> [Sai23]. <sup>3</sup> [ERVN24, Mar21, TTDT20]. <sup>31</sup> [CMG<sup>+</sup>24, FBP<sup>+</sup>22]. <sup>3</sup> $\Pi_u$  [Kop22a]. <sup>3</sup> $\Sigma_g^-$  [Kop22a].  <sup>$\beta$</sup>  [LL21b]. <sup>*I*</sup> [PAS<sup>+</sup>20]. <sup>*II*</sup> [ĆPP<sup>+</sup>22]. <sup>pro</sup> [PPP21]. <sup>tz</sup> [BVGB23]. <sup>1</sup> [Dor20, ERVN24].  <sup>$+,0,-$</sup> <sub>1,2,3</sub> [JX24]. <sup>10</sup> [LR20, LXP<sup>+</sup>22].  <sup>$+$</sup> <sub>12</sub> [PGP<sup>+</sup>23]. <sup>18</sup> [PP23]. <sup>2</sup> [AQRA<sup>+</sup>23, AQMM<sup>+</sup>23, AQIS<sup>+</sup>24, AMM22, ABAQ<sup>+</sup>23, AR20, AWK<sup>+</sup>23, BR23, DSC20, DBE20, DLH<sup>+</sup>23, DGSB<sup>+</sup>20, FP22, FP23, GGK20, GKA<sup>+</sup>23b,

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

**-1** [ZDBZ20]. **-3-3'-diol** [BBBP<sup>+23</sup>]. **-acceptor** [JGdC<sup>+23</sup>]. **-acenes** [MdSJ<sup>+23</sup>]. **-acetato** [MVP<sup>+20</sup>]. **-alanine** [DC22b]. **-alkanes** [PFPD21]. **-aminotetrazole** [JMV21]. **-aromatic** [RTB23]. **-Azacryptand** [Ari24]. **-Based** [DBE20]. **-benzoquinone** [SHH<sup>+24</sup>]. **-benzyl** [BAM<sup>+24</sup>]. **-block** [AR20]. **-bridged** [KBHG23]. **-C** [HSG21, LZW<sup>+23</sup>]. **-catalyzed** [HCY<sup>+22</sup>, LLS<sup>+22b</sup>]. **-complexes** [BKM21]. **-conjugated** [CBF<sup>+20</sup>]. **-Conjugation** [CMO<sup>+24</sup>]. **-covalency** [ZBH<sup>+23</sup>]. **-Cp** [HSG21]. **-cube** [Bal20b]. **-cyclodextrin** [IAS<sup>+24</sup>]. **-cyclopenta** [MSE<sup>+21</sup>]. **-D-Glucopyranose-silver** [Mon24]. **-dependent** [Ngo21, JRS20]. **-diaqua** [MVP<sup>+20</sup>]. **-diketones** [AV20]. **-elimination** [KZJ21]. **-F12** [CK22]. **-functions** [SCZ<sup>+21</sup>]. **-grasp** [BPDG21]. **-hairpin** [ZZ23b]. **-helical** [SSS<sup>+20b</sup>]. **-hexane** [NS22]. **-Hole** [RZS<sup>+23</sup>, JGGPN21, LK22, Sch22a, SJZ<sup>+21</sup>]. **-Hydrido** [SLML24]. **-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]. **-sheets** [XIV<sup>+</sup>24]. **-thymine** [SSS<sup>+</sup>20a]. **-TriPip222** [Ari24]. **-water** [VCRP23]. **-xTB** [OM22].

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

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

**2** [BBBP<sup>+</sup>23, MSE<sup>+</sup>21, dMBdAVdS24, 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'-bipyridyl** [BBBP<sup>+</sup>23]. **2-body** [KG23]. **2'-disulfanediybis** [MSE<sup>+</sup>21]. **2-ethenediol** [MLGY24]. **2-ethylhexanoate** [BR23]. **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** [BBBP<sup>+</sup>23, GSJ<sup>+</sup>23, VZG<sup>+</sup>24]. **3-cycloaddition** [SVTK<sup>+</sup>22]. **3-D** [GSJ<sup>+</sup>23]. **3-dienes** [BXY<sup>+</sup>24]. **3-tetrafluoro-1-propene** [BR23]. **3-trifluoro-1-nitroprop-1-ene** [SMB<sup>+</sup>23]. **3-trifluoropropene** [BR23]. **31** [dSSRVdM24]. **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, MY24, YIO20].

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

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

**7** [CM20b]. **74** [ZHG<sup>+</sup>24]. **7D** [Bal20a]. **7D-Hypercube** [Bal20a].

**8-hydroxyquinolinato** [AS20].

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

**AA** [ZWY<sup>+</sup>22]. **Ab-Initio**

[GK24, RZS<sup>+</sup>23, RPD<sup>+</sup>20a, BBBP<sup>+</sup>23, 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, KBK<sup>+</sup>24, SNK24b]. **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** [JGdC<sup>+</sup>23, PTP23, TANC23]. **Accessible** [GCL<sup>+</sup>20, VCL20]. **accuracy** [Cha24, KWX23, RMJ21, YFH<sup>+</sup>21]. **Accurate** [DKB23, Dor20, ERVN24, LRF<sup>+</sup>21, PWX<sup>+</sup>20, PYA24, Ben22, BP22, CSWW20, NDK24, 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]. **acetylcholinesterase** [AR24]. **Acetylene** [OOY20, SVTK<sup>+</sup>22, SVR<sup>+</sup>24, 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>+</sup>21]. **acidities** [Brz22]. **acidity** [MLGY24, PT21]. **acids** [CH23, PT21]. **acrylate** [MSA22a]. **actinide** [SDK20]. **Actinium** [TLS23]. **actinoids** [LJW<sup>+</sup>23]. **action** [DSS<sup>+</sup>24, SVDS21]. **Activated** [WLZM20, LYX<sup>+</sup>22]. **Activation** [BWM20, MKSS20, MGCM21, SLR<sup>+</sup>20, ABZ20b, DZL<sup>+</sup>20, FP22, KDMM24, KJV23, LA20, MC24, PRF20, SHP<sup>+</sup>23, SLML24, WW24, ZYZ24]. **Active** [VDK<sup>+</sup>20, AFR<sup>+</sup>24a, BBC20, BP22, HL20, RvWH23, TIK21, TZS<sup>+</sup>22, UR23, WS21]. **activities** [MYYS24, YFS20]. **activity** [BHR<sup>+</sup>21, KLC<sup>+</sup>24, NAAP21, SS20, DMTR22, ZMH<sup>+</sup>21]. **Acylation** [CD20]. **Ad** [FBP<sup>+</sup>22]. **Ad-MD** [FBP<sup>+</sup>22]. **adamantane** [SAZ<sup>+</sup>23]. **adamantane-like** [SAZ<sup>+</sup>23]. **adapted** [GH22b, GH23, NTK21, OE20, UR23]. **Adaptive** [DZ23, SS23, ZQ24, NSRK21]. **Adatom** [JGSA22]. **additive** [KYM20]. **additivity** [PB20]. **Adenine** [BVGB23]. **adiabaticity** [RCC<sup>+</sup>20]. **adjusted** [GH22a, VV20b]. **adsorbate** [LHB<sup>+</sup>24]. **adsorbate-substrate** [LHB<sup>+</sup>24]. **adsorbates** [KPDB22]. **Adsorption** [GGK20, FP22, FBM<sup>+</sup>23, JGSA22, SS23, YYZ<sup>+</sup>21, ZHG<sup>+</sup>24]. **advance** [SDH23]. **Advances** [DGS24, MR21, MPR22]. **Advancing** [YGG<sup>+</sup>23]. **advantage** [BPDG21]. **aeruginosa** [VDK<sup>+</sup>20]. **affinities** [PWX<sup>+</sup>20]. **Affinity** [dSBFdAJ20, DC22b, HLV<sup>+</sup>24, KZOV23, NAN<sup>+</sup>23, Ngo21, NGD22, SW21, TWT<sup>+</sup>22]. **affinity-selected** [KZOV23]. **affordable** [DKB23]. **Ag** [MH20, DA22, LZW<sup>+</sup>23, PP23]. **against** [dMBdAVdS24, EIT<sup>+</sup>21, SKL23, UAC<sup>+</sup>23]. **agent** [SDK20]. **agents** [MML<sup>+</sup>23]. **aggregate** [RDS<sup>+</sup>20]. **aggregates** [TMO<sup>+</sup>21]. **Aggregation** [DB23]. **agonist** [BRNB21]. **aided** [KGS<sup>+</sup>22]. **AIMD** [WW24]. **Al** [AS20]. **alanine** [DC22b, FP23]. **albicans** [ZOD<sup>+</sup>22]. **Alchemical** [TM20, WFBB22, BF22, GFRNC21, HB21, WdGG24, Min20]. **alcohols** [ZWY<sup>+</sup>22]. **Alder** [MNZGO<sup>+</sup>20, MGCM21, NMMC21, SSYB<sup>+</sup>20].

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

**anticancer** [DSS<sup>+</sup>24, HBM<sup>+</sup>20]. **antiferromagnetic** [Wan23].  
**antimicrobial** [SEBE21]. **antimony** [PT21]. **antioxidants** [KLC<sup>+</sup>24].  
**antiporter** [WSV20]. **antipsychotic** [dCRM21]. **antiretroviral** [CBK<sup>+</sup>24].  
**antitumor** [PRH20]. **any** [dCRM21]. **AOMadillo** [BK24]. **applicability**  
 [GH22a, LSP23]. **Application**  
 [GJMPB<sup>+</sup>20, KdILC22, MZ21, PJJL23, PHS<sup>+</sup>20, RMBSPJSG24, 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, AQIS<sup>+</sup>24, CC22, IYI<sup>+</sup>20,  
 IRB<sup>+</sup>23, KGS<sup>+</sup>21, KF24, LM24, SIW21, SKS21, SPT21, TAB<sup>+</sup>24, TCS<sup>+</sup>21a].  
**applied** [HBM<sup>+</sup>20, KCGK20, MMF<sup>+</sup>24, PMT<sup>+</sup>22]. **apply** [PDL<sup>+</sup>21].  
**Applying** [dMBdAVdS24]. **Approach**  
 [PWW20, SBG20, SB20, ARR22a, ARR22b, AAL21, ASW20, dMBdAVdS24,  
 CN21, CBK<sup>+</sup>24, ĆPP<sup>+</sup>22, DGSB<sup>+</sup>20, DOT22, HBT<sup>+</sup>20, IYI<sup>+</sup>20, IRB<sup>+</sup>23,  
 JGGPN21, KMR<sup>+</sup>24, KG23, KPHV23, KEK23, LBH<sup>+</sup>22, LL22, LDT<sup>+</sup>22,  
 MZMK<sup>+</sup>21, MJS<sup>+</sup>23, MSA22b, NMF121, OSHT20, PW20, RDB23, STR20,  
 TAC<sup>+</sup>23, TMO<sup>+</sup>21, TSR21, VCL20, WYC<sup>+</sup>24, YC23]. **approaches**  
 [AV20, CGSP24a, GH22a, PCB<sup>+</sup>24]. **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, ĆNF23, KK23, KWB24, KTM<sup>+</sup>23,  
 LGD<sup>+</sup>20, PDC23, RPD<sup>+</sup>20a, SNK24b, 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**  
 [ZWL<sup>+</sup>24a, APS20, GAP21, MAI22, ODL20, RTB23, TLD<sup>+</sup>22]. **aromaticity**  
 [BGPR24, CMO<sup>+</sup>24, DZ23, FMK24]. **art** [BSF20]. **artifacts** [ÖLP<sup>+</sup>20].  
**Artificial** [QB20, KI24, 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, PSA<sup>+</sup>23, ZRSST20].  
**assisted** [ARA22, AV20, ARR22b, CRT<sup>+</sup>21, HUUO23, KF24, KGTL21,  
 LL21b, LL22, MLC<sup>+</sup>23, RD24, WRBT21]. **association**  
 [GBM20, SSS<sup>+</sup>20b, YJZ<sup>+</sup>22]. **astatine** [PHS<sup>+</sup>20]. **astrochemical**  
 [MLGY24]. **asymmetric** [HCY<sup>+</sup>22, PRIP24]. **atom**  
 [BUNO22b, ĆNF23, DART21, DLH<sup>+</sup>23, GFRNC21, LKM20, LK22, PDC23,  
 SaATR24, SHH<sup>+</sup>23a, WMJ<sup>+</sup>22, WGKG20]. **atom-centered** [LK22]. **atomic**  
 [AÅFJ21, BP22, EVKL21, KRW<sup>+</sup>24, KWMPR24b, LL21b, MP24, 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,  
 HLV<sup>+</sup>24, JCMHT22, JGGPN21, LGM20, LGM22, LYX<sup>+</sup>22, MSYS23, MC23,  
 NTK21, NSH23, OE20, Sch22b, SG20, Wan23]. **atoms-in-molecules**  
 [MC23, NTK21]. **attack** [BA24, CRT<sup>+</sup>21]. **attraction** [IN23b]. **attractors**

[KE23b]. **augmented** [NEG<sup>+</sup>20, Pil20]. **auto** [CJHW21]. **auto-analysis** [CJHW21]. **AutoDock** [PNT<sup>+</sup>22]. **automata** [LCLB24]. **Automated** [COK22, CR24, GSD<sup>+</sup>22, WHJM23, ZLLL22, MNBG<sup>+</sup>21, RSHG23, RB22, SSMP23]. **Automatic** [SM22a, FKT21]. **automatically** [APP24]. **Automation** [WLWR22]. **Automotive** [SC23]. **Automatized** [ABNG22, SYS<sup>+</sup>21]. **AutoMeKin2021** [MNBG<sup>+</sup>21]. **auxetic** [MMAZ<sup>+</sup>23]. **auxiliary** [Fed24, MFS22, NSH23, SM22a]. **availability** [RD24]. **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]. **Azacryptand** [Ari24]. **azide** [XZZ<sup>+</sup>20]. **aziridine** [JAP<sup>+</sup>24]. **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, ERVN24, LWC<sup>+</sup>24, MIP<sup>+</sup>21]. **B3LYP** [LRF<sup>+</sup>21, SW21]. **Ba** [AQRA<sup>+</sup>23]. **BaC** [SGSB23]. **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** [PGDD24, GAP21, MA23a, MA23b, ZLLL22, LPP20]. **bandgap** [dARW<sup>+</sup>23]. **bands** [Sch22a]. **Bank** [ENR<sup>+</sup>24]. **BAR** [ZK21]. **barriers** [MML<sup>+</sup>23]. **Barshad** [VFCG20]. **base** [DDSM23, HLV<sup>+</sup>24]. **Based** [DBE20, AV20, ARR22a, BPT<sup>+</sup>23, BMA<sup>+</sup>24, BAO<sup>+</sup>20, Ben22, BEKM24, Brz23, CDCT21, CM20a, CP23, CN21, CR24, 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, HTTT23, HM21, HGR<sup>+</sup>24, JMV21, KRW<sup>+</sup>24, 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, UR23, UB20, VWP<sup>+</sup>22, VHS<sup>+</sup>24, Vyb23, WZW<sup>+</sup>24, WYC<sup>+</sup>24, XZC<sup>+</sup>24, YLZ<sup>+</sup>20, ZLLL22, ZS22, ZFRM20, dSSCC24]. **bases** [Sch22a]. **basic** [PSW<sup>+</sup>24]. **basicity** [DC22b, GSH23, MLGY24, SGRN24, SW21]. **Basis** [YXGZ20, CM20b, Fed24, GZFSM21, GH22b, GH23, HGR<sup>+</sup>24, IN23b, KM24, LB21, LB22, MFS22, MM24, MCP23, NSH23, RNP20, SLB23, SM22a, SCKH21, SM20, SCCZ21, TAC<sup>+</sup>23, WCT<sup>+</sup>23]. **basis-set** [HGR<sup>+</sup>24, TAC<sup>+</sup>23]. **bath** [CQSG20]. **batteries** [SGT<sup>+</sup>20]. **battery** [Ore24]. **Bayesian** [AVM21, LBH<sup>+</sup>22]. **Bdf1** [ZOD<sup>+</sup>22]. **Be** [ZDBZ20, BTSB22, RD24, SKKG22, YOCMA23, YMSS23]. **BEE** [AKGD24]. **BeH** [MMAZ<sup>+</sup>23]. **Behavior** [NI22, AK20, BR23, KDKS21]. **Bel** [ZXD20b, ZXD20a]. **BeM** [PTP23]. **Benchmark** [DC22b, MLP22, SW21, SC22, AZKM22, CPG21, CS20, DGSB<sup>+</sup>20, NAN<sup>+</sup>23, OMC<sup>+</sup>20, PGH24, dASRHB21]. **Benchmarking** [LSP23, LWC<sup>+</sup>24, MAKZ23, XZ20, RLHG<sup>+</sup>23, SI22]. **beneficial** [BTSB22]. **Benoît** [IBL20]. **bent** [WG20]. **benzaldehyde** [DSK21, NMMC21, SW21]. **benzene** [CMO<sup>+</sup>24, FMK24, NMFI21, RC22, XCJ20, ZS22].

**benzene-bridged** [ZS22]. **benzoin** [DSB23]. **benzoquinone** [SHH<sup>+</sup>24].  
**benzothiadiazole** [ZWL24b]. **benzyl** [BAM<sup>+</sup>24]. **benzyne** [GM22].  
**benzyne/aryne** [GM22]. **benzynes** [BGPR24]. **Beryllium**  
 [MSYS23, Kop22b, PTP23, RMS<sup>+</sup>23, SKKG22, THLC<sup>+</sup>23, ZDBZ20].  
**beryllium-doped** [ZDBZ20]. **best** [KDP<sup>+</sup>22, ZHHS21]. **between**  
 [AR24, BW22a, BAM<sup>+</sup>24, CS20, CTBB20, dSCCN21, HYA<sup>+</sup>20, KR23, Klo22,  
 KPR23, MML<sup>+</sup>23, MPP23, Min20, NTK21, PTP23, RZS<sup>+</sup>23, SMB<sup>+</sup>23,  
 SSS<sup>+</sup>20b, XIV<sup>+</sup>24]. **BFGS** [FR21]. **bias** [KSRB<sup>+</sup>21, Tik23]. **biased**  
 [DHN<sup>+</sup>21, RGGD21]. **biased/accelerated** [RGGD21]. **biasing**  
 [GVJ<sup>+</sup>22, RR22]. **bidentate** [LLKS23, TLS23]. **bidirectional**  
 [MPP23, MMAZ<sup>+</sup>23]. **bifunctional** [HBM<sup>+</sup>20]. **bilayers** [PRIP24]. **bile**  
 [WGKG20]. **bileptic** [GPM21b]. **bimetallic** [MAKZ23]. **binary** [MJS<sup>+</sup>23].  
**BinderSpace** [KZOV23]. **Binding**  
 [GOY20, KLZ<sup>+</sup>23, KPKS23, MXM20, Min20, NNT<sup>+</sup>20, SZLD20,  
 dSBFdAJ20, BRNB21, CSP20, FDD<sup>+</sup>23, GH22a, HGF20, HLV<sup>+</sup>24, IYI<sup>+</sup>20,  
 KR23, MAKZ23, MSA22a, NAN<sup>+</sup>23, NTK21, NBE<sup>+</sup>23, Ngo21, NST<sup>+</sup>20,  
 NGD22, NN20, ÖLP<sup>+</sup>20, PWX<sup>+</sup>20, RLHG<sup>+</sup>23, SWF<sup>+</sup>20, SWM<sup>+</sup>20b,  
 SSO<sup>+</sup>20, TWT<sup>+</sup>22, WKCP21, XZX<sup>+</sup>22, YIO20, ZQ24, ZOD<sup>+</sup>22]. **binuclear**  
 [KKAK23]. **bio** [AAID22]. **bio-membranes** [AAID22]. **bioactivity**  
 [MPuS<sup>+</sup>20]. **biochemical** [YWGY22]. **bioisosterism** [dMBdAVdS24].  
**Biological** [AWID<sup>+</sup>20, CKH23, CBB<sup>+</sup>21, JKK<sup>+</sup>21, JKS23, SS20]. **biology**  
 [FPMD23, IBL20]. **biomacromolecules** [LRKD23]. **biomolecular**  
 [MAKZ23]. **Biomolecules** [WZZ<sup>+</sup>20, PGH24, SH23, ZGZC20]. **biophysical**  
 [SKS21]. **bioremediation** [FPFD21]. **biosensor** [SPT21]. **biosystems**  
 [GUCCR20]. **biphenyl** [BdLC21]. **biphenylene** [RTB23]. **BIPS** [DK23].  
**bipyridyl** [BBBP<sup>+</sup>23]. **birthday** [IBL20]. **bis** [YFS20]. **bishistidyl** [FAK24].  
**bithiophene** [AST24]. **Block** [RA20, AR20, LRKD23]. **blocks** [RA20]. **Blue**  
 [HBM<sup>+</sup>20]. **BMP** [CM20b]. **BMP-2** [CM20b]. **BMP-7** [CM20b]. **BN**  
 [MdSJ<sup>+</sup>23]. **BN-** [MdSJ<sup>+</sup>23]. **BODIPY** [FB21]. **BODIPY/Aza** [FB21].  
**BODIPY/Aza-BODIPY** [FB21]. **body**  
 [BMT23, KG23, KSP21, KWMPR24b, LLZ<sup>+</sup>23, NI22, VWJ23, WFLZ23].  
**Bohmanian** [Tik23]. **Bohmanian-style** [Tik23]. **Boltzmann**  
 [BSB<sup>+</sup>24, NSRK21, RCC21, SCvW22, UYJ<sup>+</sup>24, WK21, XAD20]. **Bond**  
 [LR20, AV20, ARR22b, AD23, AKGD24, AR24, APR21, BKM21, CRT<sup>+</sup>21,  
 DK23, GH22a, HL20, HSG21, MDO<sup>+</sup>20, MLB<sup>+</sup>23, MIP<sup>+</sup>22, MC23, PDL<sup>+</sup>21,  
 Sch22b, SSS<sup>+</sup>20a, SJZ<sup>+</sup>21, SHP<sup>+</sup>23, TTT<sup>+</sup>21, XCJ20, ZMH<sup>+</sup>21].  
**bond-angle** [PDL<sup>+</sup>21]. **bond-driven** [AR24]. **bonded**  
 [DGM22, LKT21, LML<sup>+</sup>23]. **Bonding**  
 [DDSM23, FNP22, GM22, KE23b, LHG<sup>+</sup>23, MCD22, SMH21, THLC<sup>+</sup>23,  
 AV20, AWK<sup>+</sup>23, AA20, BEKM24, BGS<sup>+</sup>20, BCN22, CVGVN<sup>+</sup>20, DGM22,  
 JX24, EK20c, FDK22, FAK24, GKA<sup>+</sup>23b, GSJ<sup>+</sup>23, JC20, JGGPN21, KZ24,  
 KS24, LLKS23, LXP<sup>+</sup>22, MVP<sup>+</sup>20, MSYS23, MP23, MIP<sup>+</sup>21, NEG<sup>+</sup>20,  
 OTZW24, SM23, Tze21, WCD<sup>+</sup>23, YSMS24, ZBH<sup>+</sup>23, dBCdL20]. **bonds**  
 [Brz22, CB20, GH22a, HS23, KP21, NTK21, PTP23, SGGG22,



dASRHB21, Sch22b, SD21, WG20, ZBH<sup>+</sup>23]. **Boosting** [KN21]. **borane** [ZZG<sup>+</sup>21]. **boranylborane** [PFP<sup>+</sup>21]. **Born** [GCL<sup>+</sup>20]. **Boron** [FP22, LWC<sup>+</sup>24, MAI22, NDK24, ZYZ24, ZS22]. **boron-centered** [ZYZ24]. **boron/phosphorus** [ZS22]. **boron/phosphorus-based** [ZS22]. **boronic** [FP23]. **borylene** [DGM22]. **boryne** [KDMM24]. **both** [KCF<sup>+</sup>20, PRH20]. **bottom** [IL24]. **bottom-up** [IL24]. **boundaries** [VZG<sup>+</sup>24]. **boundary** [BSB<sup>+</sup>24, 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]. **bridge** [JGdC<sup>+</sup>23]. **bridged** [KBHG23, ZS22]. **Bridging** [HZG<sup>+</sup>20, UYJ<sup>+</sup>24, 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, NDK24, 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, IAF<sup>+</sup>24, KWX23, MPuS<sup>+</sup>20, MCP23, MCD22, PGP<sup>+</sup>23, SHP<sup>+</sup>23, VKSS24, YLZ<sup>+</sup>22, ZHHS21]. **C-NMR** [MCD22]. **C2** [FCB23]. **C22** [FCB23]. **cAAC** [GPM21b]. **Cage** [SSSA23, DSC20, GGK20]. **Cage-size** [SSSA23]. **cages** [AST24]. **CAI** [ZXD20a]. **CAI** [ZXD20b]. **calculate** [FBP<sup>+</sup>22, SS20, WFBB22]. **calculated** [ABAQ<sup>+</sup>23]. **Calculating** [KWX23]. **Calculation** [CV22, Sán20, Cha24, CSWW20, HNCL24, KM22, MR21, NML21, ÖLP<sup>+</sup>20, PRF20, RB24, SCCZ21, VCL20, VV21, YBS<sup>+</sup>20, ZQ24]. **Calculations** [DBE20, MXM20, Min20, AiIS<sup>+</sup>21, BSS<sup>+</sup>22, BSR22, CMG<sup>+</sup>24, CKH23, CLTMd<sup>+</sup>23, DGsb<sup>+</sup>20, EK20b, EPT21, FV20, FB20, GBM20, HB21, HM21, HRTSS<sup>+</sup>20, HLV<sup>+</sup>24, KL20, KK23, LB21, LB22, LWC<sup>+</sup>24, MLC<sup>+</sup>23, MAM<sup>+</sup>23, Mar21, MY24, MSA<sup>+</sup>24, 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, UR23, WdGG24]. **Calibration** [DPSG20]. **CAM** [LRF<sup>+</sup>21]. **CAM-B3LYP** [LRF<sup>+</sup>21]. **camptothecin** [PRH20]. **Can** [BTSB22, RD24, PBM21]. **cancer** [SVDS21]. **Candida** [ZOD<sup>+</sup>22]. **canonical** [GGK20, KSRB<sup>+</sup>21, ZKJ<sup>+</sup>23]. **capacity** [SKKG22]. **capped** [AST24]. **caps** [Fed24]. **capsanthin** [PSA<sup>+</sup>23]. **capture** [BBB<sup>+</sup>23, KOD21]. **carbene** [DGM22, YSMS24]. **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, BR23, 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]. **carbonic** [KI24]. **carbonyl** [FNPD22]. **carboxy** [FDK22]. **carboxy-neuroglobin** [FDK22]. **carboxyl** [CCZ23]. **carboxylate** [OSM20]. **carboxylate-promoted** [OSM20]. **carboxylates** [PCI23]. **carboxylation** [JMK<sup>+</sup>20]. **Carlo** [DMD<sup>+</sup>21, EG20, GGK20,

GNL<sup>+22</sup>, KCGK20, KEK23, PFSC20, TIK21, TMO<sup>+21</sup>, ZKJ<sup>+23</sup>].  
**Carlo/DFT** [TMO<sup>+21</sup>]. **carrier** [LHC<sup>+21</sup>, ZGZ<sup>+20</sup>]. **Cartesian**  
 [BLB20, LSCK23]. **Case**  
 [ARR22b, AA20, BEKM24, HM21, LWLC21, NPGP23, OSHT20, PDGD23,  
 RPD<sup>+20a</sup>, RCD<sup>+24</sup>, SVR<sup>+24</sup>, TMO<sup>+21</sup>, VM23]. **cases** [Ari24]. **CASPT2**  
 [TT20]. **Cassandra** [DMD<sup>+21</sup>]. **CASSCF** [LJW<sup>+23</sup>, Sts20]. **catalysis**  
 [JRS20]. **catalyst** [CJHW21, MAM21]. **catalysts**  
 [DRBT24, DLH<sup>+23</sup>, MLB<sup>+23</sup>, MKB<sup>+21</sup>, SHP<sup>+23</sup>, WKG<sup>+23</sup>]. **catalytic**  
 [CJHW21, CL23, DSK21, MKB<sup>+21</sup>, MYYS24, PFPD21, PM21, YFS20,  
 ZMH<sup>+21</sup>]. **Catalyzed**  
 [LLS<sup>+22b</sup>, AMM22, BXY<sup>+24</sup>, HCY<sup>+22</sup>, HYA<sup>+20</sup>, NMMC21, PRH20, SKY24].  
**cathode** [LCP24]. **Cation**  
 [LJ20, Kop22b, ODL20, OAN<sup>+23</sup>, 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** [AQRA<sup>+23</sup>, JS21].  
**CdSe** [LWLC21]. **Celebrating** [IBL20]. **cells** [AYO20, SZP<sup>+20</sup>, TANC23].  
**CellSys** [AAID22]. **cellular** [LCLB24, YMM<sup>+24</sup>]. **cellular-scale** [YMM<sup>+24</sup>].  
**cellulose** [LGJF22]. **center** [LK22]. **centered** [KZ24, LK22, ZYZ24].  
**CEPA/1** [Sán20]. **cesium** [GH23]. **CGeGaAl** [DC22a]. **CH**  
 [AMM22, SVTK<sup>+22</sup>, dCVARN20, BdLC21, KPTT21, MK22b, SVTK<sup>+22</sup>,  
 SLR<sup>+20</sup>, dSSRVdM24, SCC<sup>+22</sup>, WW24, XZW<sup>+21</sup>, ZHG<sup>+24</sup>, dCVARN20].  
**chain** [Shi22, SSS<sup>+20b</sup>]. **chains** [BSR22, ODL20]. **Chalcogen**  
 [MDO<sup>+20</sup>, SaATR24, 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** [AÅFJ21].  
**CHAMPION** [AÅFJ21]. **change** [JGM21, XIV<sup>+24</sup>]. **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>].  
**chapter** [SVR<sup>+24</sup>]. **character** [BGS<sup>+20</sup>, LHG<sup>+23</sup>, MLX<sup>+24</sup>, SD21].  
**characteristics** [AQRA<sup>+23</sup>, AQIS<sup>+24</sup>, 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>, PYA24, SBB<sup>+22</sup>]. **characterize** [APP24, LKK<sup>+23</sup>].  
**Charge** [GRN20, SKKK20, AST24, Ano24a, BBC<sup>+21a</sup>, JGdC<sup>+23</sup>,  
 BOPJ<sup>+21a</sup>, CPG21, CMO<sup>+24</sup>, CB20, CCPR24, IN23b, IK21, KCGK20,  
 KWB24, dCB23, NVBG23, ÖLP<sup>+20</sup>, Ore24, 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>, CCPR24, IK21]. **charged** [HPG20, SSP23]. **charges**  
 [CX21b, LK22, MM24, NEG<sup>+20</sup>]. **Charm** [WMZJ20]. **CHARMM**  
 [BTL24, FVSS20, KLP<sup>+22</sup>, KYM20, QLC<sup>+20</sup>, TPB22, VWP<sup>+22</sup>].

**CHARMM-based** [VWP<sup>+</sup>22]. **CHARMM-GUI** [KLP<sup>+</sup>22, QLC<sup>+</sup>20].  
**Chem** [MT20a, WG21, CSG<sup>+</sup>21]. **chemcoord** [WHJM23]. **Chemical**  
 [AWK<sup>+</sup>23, AWID<sup>+</sup>20, BEKM24, CGMRVBAl22, DF22, MSL<sup>+</sup>20, OoY20,  
 PAS<sup>+</sup>20, VAL20, WG21, AKGD24, APR21, BHR<sup>+</sup>21, Ben22, BBK<sup>+</sup>21,  
 CKH23, CP23, CSG<sup>+</sup>21, CB20, DGS24, DGsb<sup>+</sup>20, EK20c, HGF20, JAP<sup>+</sup>24,  
 KWX23, KFLP21, KB22, LT23, LC22, MLC<sup>+</sup>23, MH22, MN20, MAI22,  
 MPV22, NEG<sup>+</sup>20, OKI<sup>+</sup>21, PHS<sup>+</sup>20, Pil20, RSHG23, SBFSJMLU23, SIW21,  
 SYS<sup>+</sup>21, SC23, SR23, SKT24, SCC<sup>+</sup>22, TANC23, TTDT20, Tze21, UB20,  
 VWJ23, Wan21a, Wan21b, WHJM23, YGG<sup>+</sup>23, ZHHS21].  
**chemical-bonding** [NEG<sup>+</sup>20]. **chemically** [BUNO22b, BP22, TCS<sup>+</sup>21a].  
**chemicals** [CSG<sup>+</sup>21, WRVP22]. **Chemisorption** [PKT21]. **chemistry**  
 [BBB<sup>+</sup>23, DKB23, GP21, KRSD<sup>+</sup>23, KBK<sup>+</sup>24, LGM20, NVBG23, PSGL21,  
 SDK20, SSMP23, SNN<sup>+</sup>21, TPD21, TLS23, TCS<sup>+</sup>21a, TV22, TSH<sup>+</sup>23,  
 VAP<sup>+</sup>21, XSP<sup>+</sup>23]. **chemoselectivity** [SLML24]. **Chignolin** [ZZ23b].  
**ChimeraX** [SIW21]. **chiral**  
 [GJMPVR<sup>+</sup>20, MNZGO<sup>+</sup>20, MLX<sup>+</sup>24, PFP<sup>+</sup>21, SRB21]. **chirality**  
 [PPFL23]. **chloride** [Mil21]. **chloro** [BR23]. **choice** [SCKH21]. **Cholesterol**  
 [Ban20]. **chromophore** [RPD<sup>+</sup>20a]. **chromophores** [BSR22, MSA22b]. **CI**  
 [CN21, Gie21, UR23]. **CIFDock** [VWP<sup>+</sup>22]. **circuit** [KF24]. **circular**  
 [MSA22b]. **Cis** [YXGZ20]. **Cis-Azobenzene** [YXGZ20]. **Cl**  
 [SCC<sup>+</sup>22, ZG21, ABAQ<sup>+</sup>23, BEKM24, 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** [CGMRVBAl22]. **closed**  
 [GSSG24, Klo22, MB21, SM23]. **closed-shell** [GSSG24, Klo22, MB21].  
**Cluster** [BLP20, WZZ<sup>+</sup>20, BtSB22, BSF20, DC22b, FB21, GRBN21,  
 HPM<sup>+</sup>21, KPDB22, KTBS23, LWC<sup>+</sup>24, MMF<sup>+</sup>24, NSKN21, SKKG22,  
 SAZ<sup>+</sup>23, STR20, WP20, ZWL<sup>+</sup>24a]. **cluster-continuum** [STR20]. **Clusters**  
 [MFC20, AD23, AKGD24, 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, OM22, OM23, POPGS22, RDB23, TT20, TSR21, VTdlM20,  
 WMJ<sup>+</sup>22, Wan23, WZW<sup>+</sup>24, XDZ23, YOCMA23, ZDBZ20]. **Cm** [LJW<sup>+</sup>23].  
**CO** [BR23, PTP23, WLZM20, LXP<sup>+</sup>22, DZL<sup>+</sup>20, GKA<sup>+</sup>23b, MSA22a,  
 AMM22, AR20, Ano24a, DGsb<sup>+</sup>20, FP22, FP23, FDK22, JAP<sup>+</sup>24, LHC<sup>+</sup>21,  
 MC24, MK22b, RC22, SK23, SBB<sup>+</sup>22, SLML24, VCRP23, WP20, XLW<sup>+</sup>22,  
 YYZ<sup>+</sup>21, MYYS24]. **co-deposition** [MSA22a]. **co-factor** [GKA<sup>+</sup>23b].  
**CO-N** [XLW<sup>+</sup>22]. **coagulants** [RD24]. **Coarse**  
 [MT20a, WSL<sup>+</sup>20, WZZ<sup>+</sup>20, BS23, CST23, GWN21, IL24, KGTL21, LL21b,  
 LL22, MT19, SSDL<sup>+</sup>23, XZC<sup>+</sup>24]. **Coarse-Grained**  
 [MT20a, WSL<sup>+</sup>20, WZZ<sup>+</sup>20, BS23, CST23, GWN21, IL24, KGTL21, LL21b,  
 LL22, MT19, SSDL<sup>+</sup>23]. **coarse-to-fine** [XZC<sup>+</sup>24]. **cobalt** [HCY<sup>+</sup>22].  
**COBRAMM** [ABNG22, CMG<sup>+</sup>24]. **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, YSMS24]. **Colab** [PSW<sup>+</sup>24]. **coli** [CGSP24a]. **collective** [BPT<sup>+</sup>23]. **collective-variable** [BPT<sup>+</sup>23]. **collision** [BBY<sup>+</sup>21]. **Colorings** [Bal20a]. **combination** [GVJ<sup>+</sup>22, KK23]. **Combined** [RMJ21, AiIS<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** [AiIS<sup>+</sup>21]. **Comparative** [JMV21, PM21, BA24, SGRN24, THH<sup>+</sup>24]. **compared** [LML<sup>+</sup>23, WD20]. **Comparing** [CCHS23]. **Comparison** [BSS<sup>+</sup>22, CN21, NUK21, RLHG<sup>+</sup>23, SK20, WK21, Ano24a, DGM22, GG22, HSG21, SVTK<sup>+</sup>22, SK23]. **compatible** [BTL24, PLP<sup>+</sup>20]. **competing** [ČNF23]. **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, Mon24, OE20, SWF<sup>+</sup>20, SIW21, SC23, TM20, WHJM23, YYS20, ZMH<sup>+</sup>21, ZZG<sup>+</sup>21]. **complexation** [SGRN24, SDK20]. **Complexes** [AD20, BGS<sup>+</sup>20, ASL<sup>+</sup>20, AS23, AS20, Ari24, BKM21, Brz22, CL23, CMD<sup>+</sup>22, ČPP<sup>+</sup>22, DGM22, DSK21, FNP22, GKA<sup>+</sup>23b, GP21, Jab22a, KMR<sup>+</sup>24, KK23, KBHG23, KKAK23, KDP<sup>+</sup>22, LLKS23, LKT21, LZW<sup>+</sup>23, LML<sup>+</sup>23, MNH21, MVP<sup>+</sup>20, MLM<sup>+</sup>24, MGB<sup>+</sup>22, MYYS24, MCD22, NBE<sup>+</sup>23, PTP23, PB20, PLT24, PP23, RLHG<sup>+</sup>23, SVDS21, SEZ20, SD21, THLC<sup>+</sup>23, WYC<sup>+</sup>24, XZX<sup>+</sup>22, YFS20, YSMS24, dBCdL20]. **component** [IWN24, KWYN23, KL20]. **components** [AV20, NTK21]. **composite** [CK22, PW20, PCB<sup>+</sup>24, SFS24]. **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, dMBdAVdS24, KBK<sup>+</sup>24, MAI22, MCP23, MP23, NI22, NPGP23, PDGD22, PDGD23, PHS<sup>+</sup>20, QLW<sup>+</sup>22b, SW21, SS24].

**Comprehensive** [SS24, YIO20, JGdC<sup>+</sup>23, PRH20, ZK23]. **compressed** [XZZ<sup>+</sup>20]. **compression** [CC22]. **Comput** [MT20a, WG21]. **Computation** [ALA20, CM20a, GZFSM21, MN20, SZL23]. **Computational** [ARA22, AD20, AR20, BW22a, ČNF23, GOY20, KZP22, KMR<sup>+</sup>24, KJV23, KBHG23, MPV22, Sai23, SKGG23, XZ20, ZMH<sup>+</sup>21, CGSP24a, CBK<sup>+</sup>24, CRT<sup>+</sup>21, DSS<sup>+</sup>24, JC20, KZJ22, KPHV23, LCP21, MDO<sup>+</sup>20, MK22a, MSA22b, NMMC21, Ore24, 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, MM24, 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, KWMPR24b, MPP23, POvG21].

**concentrations** [CX21b]. **conceptual** [ČPP<sup>+</sup>22, GD23, MGCM21].

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

[Ano24a, ASW20, BJ22, DYGM21, HGR<sup>+24</sup>, NI22, VL22].  
**correction-scaling** [ASW20]. **Corrections** [HFPS20, POPGS22].  
**correlated** [SM22a]. **Correlation** [NSH23, AA20, HM21, MH22, MPR22, MM24, NTK21, PW20, RMJ21, Sán20, SPSH20, SSO<sup>+20</sup>, TV22].  
**correlations** [AS20, YW20]. **corresponding** [HSG21]. **corrole** [ASL<sup>+20</sup>].  
**COSMO** [GSH23, SHHH22, VAL20]. **COSMO-RS** [SHHH22, VAL20].  
**cosolvent** [TTH<sup>+21a</sup>]. **cost** [CK22, DKB23, KWX23]. **costly** [CSWW20].  
**Coulomb** [CQSG20]. **coumarin** [ZRSST20]. **coumarin-schiff** [ZRSST20].  
**Counterion** [SLR<sup>+20</sup>, LCLB24]. **counterparts** [NG20]. **counterpoise** [NI22].  
**Coupled** [BWM20, BS23, BTSB22, BSF20, ČNF23, DC22b, FB21, GRBN21, HPM<sup>+21</sup>, RCC<sup>+20</sup>, RDB23, WGKG20, WdGG24, XCJ20].  
**coupled-cluster** [BSF20, DC22b]. **Coupling** [BSB<sup>+24</sup>, ABZ20b, AMM22, DZL<sup>+20</sup>, FCPG20, HCY<sup>+22</sup>, IMT<sup>+21</sup>, MML<sup>+23</sup>, POPGS22, Tou21, Wan23].  
**couplings** [SBD<sup>+21</sup>, SCKH21]. **COV** [ONA<sup>+20</sup>, dMBdAVdS24, EIT<sup>+21</sup>, KLZ<sup>+23</sup>, PDC23, PPP21, PPRS22, SLMA21, YC23, UAC<sup>+23</sup>]. **CoV-2** [UAC<sup>+23</sup>].  
**covalency** [ZBH<sup>+23</sup>]. **Covalent** [AWID<sup>+20</sup>, GSJ<sup>+23</sup>, SKT24].  
**Cover** [AFR<sup>+24b</sup>, 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>+21b</sup>, BOPJ<sup>+21b</sup>, CX21a, CGSP24b, ETT21a, GPM21a, GKA<sup>+23a</sup>, HAC<sup>+23a</sup>, KE23a, KFTB20a, KSS21a, KWMPR24a, KK22b, MLG<sup>+21a</sup>, QLW<sup>+22a</sup>, RPD<sup>+20b</sup>, SWM<sup>+20a</sup>, dRHB21, SNK24a, SSFS22a, TTH<sup>+21b</sup>, TCS<sup>+21b</sup>, VV20a, WTST24b, WLSC23b]. **coverages** [VHS<sup>+24</sup>]. **COVID** [SLMA21].  
**COVID-19** [SLMA21]. **Cp** [HSG21, WLZM20]. **CR** [WLZM20, MYYS24, Wan23, XDZ23]. **Cr-doped** [XDZ23]. **create** [ZK23].  
**created** [ARR22a]. **creating** [LKM20]. **Criegee** [SK20]. **Critical** [SB20, dSCCN21, MT20b]. **CrMnSi** [WZW<sup>+24</sup>]. **cross** [ABZ20b, ALA20, CV22, KGTL21, ZK23, dBCdL20]. **cross-coupling** [ABZ20b]. **cross-link-assisted** [KGTL21]. **cross-platform** [ZK23].  
**cross-sections** [CV22, dBCdL20]. **crossing** [SaATR24, WTST24a]. **crucial** [KE23b, MBBU23]. **cryo** [LSP23, PJJL23, Yos24]. **cryo-electron** [Yos24].  
**cryo-EM** [LSP23, PJJL23]. **Crystal** [GLC<sup>+22</sup>, SGSB23, AK20, CX23, KZP22, MZ21, RDS<sup>+20</sup>]. **crystallin** [FLT23]. **Crystalline** [HZG<sup>+20</sup>, Cer22, PDGD22]. **crystals** [BEKM24, LT23, LWF<sup>+22</sup>, NMF121]. **Cs** [SL20, AQIS<sup>+24</sup>, BEKM24].  
**CSiGaAl** [DC22a]. **CsPbBr** [BBL<sup>+22</sup>]. **Cu** [MH20, AD20, JGSA22, LZW<sup>+23</sup>, PP23, SPSH20]. **cube** [Bal20b]. **cupric** [XZZ<sup>+20</sup>]. **Current** [BSL20, SPT21, SZL23]. **Current-Flow** [BSL20].  
**Curvature** [MA23a, PRIP24]. **Curvature-weighted** [MA23a]. **cut** [WKL22]. **cut-offs** [WKL22]. **cutoff** [DO20]. **cyanomethylation** [DSK21].  
**cycle** [Dor20, MKB<sup>+21</sup>]. **cyclin** [TWT<sup>+22</sup>]. **cyclin-dependent** [TWT<sup>+22</sup>].  
**cyclization** [TYZ20]. **Cycloaddition** [LSC24, BAM<sup>+24</sup>, KZJ22, MGCM21, NMMC21, SVTK<sup>+22</sup>, SMB<sup>+23</sup>].

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

**D** [BBY<sup>+</sup>21, DF22, FLT23, GSJ<sup>+</sup>23, Mon24, 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]. **darunavir** [CBK<sup>+</sup>24]. **Data** [BK22, ENR<sup>+</sup>24,  
 SK20, TV22, XZ20, BMT<sup>+</sup>21, GG22, IMT<sup>+</sup>21, LL22, RD24, SWLC22].  
**Data-driven** [TV22]. **database** [AZKM22, CBB<sup>+</sup>21, LRKD23, GLC<sup>+</sup>22].  
**databases** [LGD<sup>+</sup>20, ZK23]. **datasets** [KZOV23, VT24]. **Dative**  
 [PTP23, YSMS24]. **daunting** [DRBT24]. **DD** [CD20]. **DD-peptidase**  
 [CD20]. **deacylation** [CD20]. **deal** [DWSX20]. **Deciphering** [HD21].  
**decker** [AS23]. **Decoding** [MIP<sup>+</sup>22, OTZW24]. **decomposed** [NVBG23].  
**decomposition** [AV20, AK20, CL23, HUUO23, JCMHT22, LHG<sup>+</sup>23,  
 MSA<sup>+</sup>24, MGCM21, MT20b, OTZW24, SSM21, TSZ<sup>+</sup>21, YMM<sup>+</sup>24, ZG21].  
**decomposition-based** [MT20b]. **decoration** [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, PGDD24, 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, MG24]. **delta**  
 [HNCL24]. **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, DRBT24, DZL<sup>+</sup>20, DOT22,  
 EPT21, FB20, GH22a, GD23, GAP21, HTTT23, HM21, HGR<sup>+</sup>24, HCS<sup>+</sup>20,  
 HLV<sup>+</sup>24, IYI<sup>+</sup>20, IW24, KZJ21, KS21, KdILC22, LRF<sup>+</sup>21, LSC24, 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,  
 OTZW24, OE20, OMC<sup>+</sup>20, OAN<sup>+</sup>23, PCB<sup>+</sup>24, PDP<sup>+</sup>24, 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-based** [HTTT23, HGR<sup>+</sup>24]. **density-fitted** [BSF20].  
**density-fitting** [HGR<sup>+</sup>24]. **Density-functional**  
 [TANC23, BWS20, NEG<sup>+</sup>20]. **density-matrix** [IW24]. **Depend**  
 [BWM20, BA24]. **Dependence** [JK21, YXGZ20, MH20, SBD<sup>+</sup>21].

**dependencies** [BK22]. **Dependent** [YXGZ20, BA22, CPG21, FB20, FNY21, IYI<sup>+</sup>20, IN23a, JRS20, MFS22, MSS20, Nan24, Ngo21, OMC<sup>+</sup>20, OAN<sup>+</sup>23, 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, CMO<sup>+</sup>24, CCPR24, JAP<sup>+</sup>24, KLC<sup>+</sup>24, KK22c, SEBE21, SGGG22, DMTR22, SM23, TANC23, ZWL24b]. **Dermocybin** [RPA<sup>+</sup>24]. **describe** [GAP21, IK21]. **described** [KKAK23]. **Describing** [HPM<sup>+</sup>21, MH22, RLHG<sup>+</sup>23]. **Description** [BLP20, HRT<sup>+</sup>20, XCJ20, ZLLL22]. **descriptor** [CMO<sup>+</sup>24]. **descriptors** [BHR<sup>+</sup>21, CMD<sup>+</sup>22, COK22, GJMPVR<sup>+</sup>20, HBT<sup>+</sup>20, LGM20, LGM22, NTK21, PDP<sup>+</sup>24, TCS<sup>+</sup>21a, YGG<sup>+</sup>23]. **Design** [IW23, PAS<sup>+</sup>20, SEBE21, BXY<sup>+</sup>24, BBB<sup>+</sup>23, CBK<sup>+</sup>24, DSK21, GLC<sup>+</sup>22, HKFT21, KI24, 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]. **detection** [CR24]. **determinant** [BTSB22]. **Determination** [NNT<sup>+</sup>20, CST23, FKT21, LHB<sup>+</sup>24]. **determines** [HYA<sup>+</sup>20]. **Determining** [WZZ<sup>+</sup>20, KPHV23, SFS24, VHS<sup>+</sup>24]. **deterministic** [TS21]. **Developing** [HKFT21]. **Development** [AFR<sup>+</sup>24a, BTL24, IL24, KG23, KTBS23, 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, Cha24, CL23, DK23, DSK21, FCB23, FBM<sup>+</sup>23, FV20, HS22, JAP<sup>+</sup>24, JMV21, KMR<sup>+</sup>24, KLC<sup>+</sup>24, KKAK23, LCC<sup>+</sup>21, LT23, LLJ<sup>+</sup>24, LDT<sup>+</sup>22, MPOC21, MJS<sup>+</sup>23, MCD22, MK22b, NG20, PLT24, RLHG<sup>+</sup>23, SVDS21, dSSCC24, SB20, SLML24, TANC23, TAB<sup>+</sup>24, TMO<sup>+</sup>21, WD20, WS21, WKG<sup>+</sup>23, YC23, ZRSST20, ZDBZ20]. **DFT-based** [dSSCC24]. **DFT-D4** [NG20]. **DFT/MRCI** [ZRSST20]. **Di-** [KZP22]. **diagnostic** [SD21]. **diagonalization** [BMT23, MB21, WFLZ23]. **diagonalization-free** [MB21]. **diagrammatic** [HD21]. **diagrams** [PDC23, SGSB23, VFCG20]. **dianionic** [DPSG20]. **diaqua** [MVP<sup>+</sup>20]. **diatomic** [AA20, Tze21]. **diatomics** [KW22]. **diazadiboretidine** [NHFS21]. **diborane** [SLML24]. **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** [MLM<sup>+</sup>24, RMS<sup>+</sup>23]. **Diels** [MNZGO<sup>+</sup>20, MGCM21, NMMC21, SSYB<sup>+</sup>20]. **diene** [NMMC21]. **dienes** [BXY<sup>+</sup>24]. **differences** [WFBB22]. **different** [JGdC<sup>+</sup>23, DO20, DWSX20, KK23, Sts20, WS21]. **differential** [SD21]. **differently** [AST24]. **diffuse** [MCP23]. **diffusion** [BUNO22b, CGMRVBAl22, FNY21, PFSC20, RGGD21, SM22b, UKBD23]. **diffusion-controlled** [CGMRVBAl22]. **diffusivity** [NS22]. **difluoro** [SKGG23]. **difluorocarbene** [ZS22]. **difluoromethane** [BR23]. **digestion** [Nee23]. **dihalogens** [RZS<sup>+</sup>23]. **dihedral** [RR22]. **Diimides** [NRH<sup>+</sup>20]. **diimine** [WCD<sup>+</sup>23]. **diketones** [AV20]. **diketopyrrolopyrrole** [dCB23]. **dimensional**



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

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

**E-fields** [AMF<sup>+20</sup>]. **E4** [WS21]. **earth** [ZWL<sup>+24a</sup>]. **earth-doped** [ZWL<sup>+24a</sup>]. **ebsele**n [YC23]. **EDA** [DGM22, GM22, GKA<sup>+23b</sup>, SM23]. **EDA-NOCV** [DGM22, GM22, GKA<sup>+23b</sup>, SM23]. **edge** [CS23]. **Effect** [AD20, DLH<sup>+23</sup>, GRN20, JC20, ARR22a, BMA<sup>+24</sup>, CBF<sup>+20</sup>, DO20, FMK24, FVSS20, JMK<sup>+20</sup>, KPHV23, KEK23, LK22, LLZ<sup>+23</sup>, MAM21, MEKH22, dCB23, PRH20, SaATR24, 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>, JGdC<sup>+23</sup>, BAM<sup>+24</sup>, CMG<sup>+24</sup>, CMO<sup>+24</sup>, CX21b, FBP<sup>+22</sup>, GCP22, GAG20, KWYN23, LCLB24, dCB23, MCD22, PCI23, SSSA23, WCY<sup>+24</sup>, dCVARN20]. **efficiency** [FYIO23, ZWL24b]. **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, RD24, TAB<sup>+24</sup>, ZQ24, ZZG<sup>+21</sup>]. **efflux** [CGSP24a]. **effort** [POvG21]. **eigenvalues** [KDLP21]. **Eighth** [PSMPB21]. **Eighth-Shell** [PSMPB21]. **elacestrant** [CSP20]. **elastic** [KOD21, LM24, MA23a, MA23b, MMAZ<sup>+23</sup>, ZLLL22]. **Electric** [PL22, SHM<sup>+20</sup>, ZG21]. **electride** [Ari24, DSC20]. **electrocatalysts** [AR20]. **electrochemical** [KDLP21, KF24]. **Electrocyclization** [PC21]. **electrode** [DOT22]. **electrolyte** [LEP<sup>+21</sup>]. **electrolytes** [EG20, HM21]. **Electron** [KZJ22, BJ22, BBC<sup>+21a</sup>, ČNF23, EVKL21, EPT21, IN23a, KZJ21, LKT21, LKAT22, LT23, MH22, MAM21, PTP23, PDP<sup>+24</sup>, RCC<sup>+20</sup>, RNP20, RTB23, SS20, SPSH20, SMB<sup>+23</sup>, SSO<sup>+20</sup>, SZL23, TAC<sup>+23</sup>, Yos24, ZYZ24, dBCdL20]. **electronegativity** [Vyb23]. **Electronic** [DGsb<sup>+20</sup>, JX24, SBFSJMLU23, SM22b, SCKH21, TT20, AQIS<sup>+24</sup>, ABAQ<sup>+23</sup>, Ari24, AMF<sup>+20</sup>, BMA<sup>+24</sup>, BTsb22, CC22, CCPR24, HSG21, IK21, JMV21, KWYN23, KPDB22, Kop22a, LM24, 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>, SS24, SGT<sup>+20</sup>, STB<sup>+20</sup>, TPZ<sup>+20</sup>, TSH<sup>+23</sup>, UR23, VM23, WMJ<sup>+22</sup>, XZW<sup>+21</sup>, XDZ23]. **electrons** [MP23, PDGD23]. **electrooxidation** [DOT22]. **electrophilicities** [HBT<sup>+20</sup>]. **Electrophilicity** [PC23]. **electrostatic** [AS20, HS23, JGGPN21, KS24, LWLC21, LDT<sup>+22</sup>, MMK<sup>+20</sup>, ÖLP<sup>+20</sup>, UB20, VL22, ZZ23a]. **Electrostatically** [TSR21]. **Electrostatics** [HRT<sup>+20</sup>, BSB<sup>+24</sup>, SCvW22, YFH<sup>+21</sup>]. **element** [BSB<sup>+24</sup>, 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** [BVGB23, LLJ<sup>+24</sup>, 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, KBK<sup>+24</sup>]. **emitters** [LYX<sup>+22</sup>]. **Emodin** [RPA<sup>+24</sup>]. **Empirical** [LJ20, KB22, PWX<sup>+20</sup>, PNT<sup>+22</sup>, RLHG<sup>+23</sup>]. **employing** [MAI22]. **enable** [BTC24]. **enabled** [BCN22, LBH<sup>+22</sup>]. **Enabling** [ENR<sup>+24</sup>]. **Enantiomerization** [LLJ<sup>+24</sup>]. **enantiomers** [IAS<sup>+24</sup>]. **enantioselective** [IAS<sup>+24</sup>]. **enantioselectivities** [BXY<sup>+24</sup>]. **Encapsulation** [CBF<sup>+20</sup>, DSC20, SSSA23]. **Encoding** [GJMPB<sup>+20</sup>]. **End** [MXM20, Ano24a, SK23, TANC23, TTK23]. **end-group** [TANC23]. **end-on** [Ano24a, SK23]. **End-Point** [MXM20, TTK23]. **ended** [GSD<sup>+22</sup>]. **ending** [SVR<sup>+24</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, LWC<sup>+24</sup>, PYA24]. **energetically** [NSKN21]. **Energetics** [HHL<sup>+20</sup>, NG20, NDK24, 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>, KRW<sup>+24</sup>, KPHV23, LCC<sup>+21</sup>, MPP23, MLB<sup>+23</sup>, MEKH22, MCP23, NTK21, ÖLP<sup>+20</sup>, OM22, PRF20, PFSC20, PGH24, TTK23, TTT<sup>+21</sup>, VV21]. **Energy** [FKT21, GRN20, KPR23, LPP20, MXM20, Min20, NNT<sup>+20</sup>, SZLD20, YYS20, APP24, AV20, ARR22a, AKGD24, AQRA<sup>+23</sup>, AK20, AA20, BBC20, BJ22, BBC<sup>+21a</sup>, BF22, CC22, CSGVF<sup>+20</sup>, CdSB<sup>+21</sup>, CSWW20, CSP20, DC22a, ERVN24, GH22a, GBM20, GVJ<sup>+22</sup>, HB21, HBM<sup>+20</sup>, HNCL24, HPM<sup>+21</sup>, JK21, JCMHT22, JGM21, KG23, KK23, KFTB20b, Kop22b, Kos22, LM24, LPF<sup>+23</sup>, LWF<sup>+22</sup>, LML<sup>+23</sup>, LHG<sup>+23</sup>, MML<sup>+23</sup>, MN20, MSL<sup>+20</sup>, MSA<sup>+24</sup>, MGCM21, MBBU23, NUK21, NTK21, NMFI21, NI22, NML21, OTZW24, OKI<sup>+21</sup>, PPV<sup>+21</sup>, PDC23, PCB<sup>+24</sup>, RDB23, RH21, Sán20, SSS<sup>+20a</sup>, SY21, SDH23, Sts20, SCCZ21, SHH<sup>+23b</sup>, SHH<sup>+23a</sup>, TWT<sup>+22</sup>, TSZ<sup>+21</sup>, THH<sup>+24</sup>, TM20, TAB<sup>+24</sup>, TSH<sup>+23</sup>, VL22, Vyb23, WTST24a, WCT<sup>+23</sup>, WFBB22, WdGG24, XLW<sup>+22</sup>, XZC<sup>+24</sup>, YBS<sup>+20</sup>, YFH<sup>+21</sup>, ZQ24, ZK21]. **energy-adjusted** [GH22a]. **Energy-based** [FKT21, LWF<sup>+22</sup>]. **energy-efficient** [TAB<sup>+24</sup>]. **energy-related** [CdSB<sup>+21</sup>]. **enforced** [WCD<sup>+23</sup>]. **engineering** [SZP<sup>+20</sup>]. **enhance** [YYZ<sup>+21</sup>]. **Enhanced**

[FMFG20, OC23, WLSC23a, BPT<sup>+</sup>23, DWSX20, KLZ<sup>+</sup>23, LGC21, MH20, MMAZ<sup>+</sup>23, ONA<sup>+</sup>20]. **Enhancement** [MSA<sup>+</sup>24]. **enol** [LKAT22]. **enrichments** [KDP<sup>+</sup>22]. **ensemble** [HTFY21, HBM<sup>+</sup>20, QLC<sup>+</sup>20, RD23, WYC<sup>+</sup>24, XLW<sup>+</sup>22]. **ensembles** [NML21]. **entangled** [WKD<sup>+</sup>21]. **entanglement** [dSSCC24]. **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** [AR24, DPSG20]. **ePharmer** [MLG<sup>+</sup>21b]. **epidermal** [BHR<sup>+</sup>21]. **EPISOL** [CKH23]. **epoxides** [WKG<sup>+</sup>23]. **equalization** [Vyb23]. **equation** [BSB<sup>+</sup>24, NSRK21, Nan24, RCC21, SCvW22]. **equations** [MB21, MT20b]. **equatorial** [SVDS21]. **equilibria** [CM20a, CA22]. **Equilibrium** [dSCCN21, KS21, MMF<sup>+</sup>24, SFS24]. **equivalent** [KF24]. **Erratum** [MT20a]. **error** [KM22, UKBD23]. **ESCASA** [LL21b]. **Escherichia** [CGSP24a]. **ESES** [UYJ<sup>+</sup>24]. **essential** [GLC<sup>+</sup>22]. **establish** [RCC<sup>+</sup>20]. **Establishing** [LWC<sup>+</sup>24]. **estimate** [LRKD23]. **estimates** [AD23, CR24]. **Estimating** [LBH<sup>+</sup>22, Ngo21, BK22]. **estimation** [AKGD24, JGM21, KZP22, KG23, LL21b, TTK23]. **Estimations** [TTT<sup>+</sup>21]. **estimator** [AZKM22, Vyb23]. **estrogen** [CSP20]. **ethane** [MLX<sup>+</sup>24]. **ethanol** [KGS<sup>+</sup>22]. **ethenediol** [MLGY24]. **ethyl** [MIP<sup>+</sup>22]. **ethylene** [HCY<sup>+</sup>22, MYYS24, MCD22, PLZT23, SVTK<sup>+</sup>22, SJZ<sup>+</sup>21]. **ethylenediamine** [MIP<sup>+</sup>22]. **ethylhexanoate** [BR23]. **ETS** [SBB<sup>+</sup>22]. **ETS-NOCV-based** [SBB<sup>+</sup>22]. **Eu** [ALA<sup>+</sup>22]. **Eulerian** [UYJ<sup>+</sup>24]. **europium** [HRTSS<sup>+</sup>20]. **Evaluating** [dSSCC24, 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]. **even** [RD24]. **events** [RLR<sup>+</sup>20, RD23, VZG<sup>+</sup>24, WRBT21]. **evidence** [CNF23]. **Evolution** [GJL21, MM20, CG20, CCPR24, DLH<sup>+</sup>23, KdLc22, 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, MM24, RMJ21, RR22, SEZ20, TV22, VV20b, XZX<sup>+</sup>22, YW20]. **exchange-** [MM24]. **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, AST24, Ari24, BGPR24, BMT23, CG20, CPG21, FCB23, FB21, FMK24, Gie21, HD21, HPM<sup>+</sup>21, IK21, JCMHT22, KL20, KWB24, LHH<sup>+</sup>21, OSHT20, OMC<sup>+</sup>20, OAN<sup>+</sup>23, 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]. **experiment** [THH<sup>+</sup>24]. **experimental** [AZKM22, BMT<sup>+</sup>21, GG22, HBT<sup>+</sup>20, HLV<sup>+</sup>24].

**experiments** [Yos24]. **Explainable** [KI24]. **Explicit** [MGB<sup>+</sup>22, CCHS23, LKT21, PGH24, RPD<sup>+</sup>20a, WLSC23a]. **explicit-implicit** [RPD<sup>+</sup>20a]. **explicitly** [LRKD23, SM22a]. **Exploration** [GVJ<sup>+</sup>22, OY20, RKC21, LGJF22, LLKS23, OC23, OKI<sup>+</sup>21, RSHG23, SDK20, San21]. **Explorer** [SSFS22b]. **Exploring** [AVM21, MSL<sup>+</sup>20, NTK21, SGRN24, SCCZ21, THH<sup>+</sup>24, YC23]. **expressed** [HCS<sup>+</sup>20]. **expression** [UKBD23]. **Extended** [GX20, RGD21, BPT<sup>+</sup>23, DWSX20, KGD<sup>+</sup>21, NBE<sup>+</sup>23, PSMPB21, KWX23]. **Extending** [PGH24]. **Extension** [AYO20, JCMHT22]. **External** [GD23, BW22b]. **extraction** [ENR<sup>+</sup>24]. **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, Cha24, 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, AiS<sup>+</sup>21, CRT<sup>+</sup>21, JCMHT22, MY24, MLX<sup>+</sup>24, MSS20, NML21, RB22, TSZ<sup>+</sup>21, YLZ<sup>+</sup>20, ZZ23a]. **fate** [CSG<sup>+</sup>21]. **FCclasses3** [CS23]. **FCI** [dSSRVdM24]. **Fe** [HSG21, IK21, LXP<sup>+</sup>22, SM22b, MYYS24, ZFRM20]. **Fe-C** [ZFRM20]. **Features** [SHM<sup>+</sup>20]. **featuring** [ZMH<sup>+</sup>21]. **FeO** [HUUO23]. **FePS** [EK20b]. **FePSe** [EK20c]. **Fermi** [ASW20]. **ferrimagnets** [WZW<sup>+</sup>24]. **ferrocenium** [CS20]. **Feshbach** [BBY<sup>+</sup>21]. **FFLUX** [HRT<sup>+</sup>20, KSP21, MP24]. **FFParam** [KYM20]. **FGFR3** [MKSS20]. **FH** [TTT<sup>+</sup>21]. **Field** [BAC20, LJ20, WSL<sup>+</sup>20, ALA<sup>+</sup>22, BJ22, BTL24, CV22, CTPJH22, FVSS20, GKO<sup>+</sup>22, IW24, KLP<sup>+</sup>22, KYM20, LRqG<sup>+</sup>22, MT21, MAKZ23, ODL20, PLP<sup>+</sup>20, PL22, SPSH20, TPB22, VHS<sup>+</sup>24, 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]. **fine** [XZC<sup>+</sup>24]. **fingerprinting** [KI24]. **fingerprints** [SKL23]. **finite** [BSB<sup>+</sup>24]. **First** [DBE20, EPT21, KDKS21, LM24, AWK<sup>+</sup>23, BRNB21, DLH<sup>+</sup>23, EK20b, KPKS23, PM21, SS24]. **First-Principles** [DBE20, KDKS21, DLH<sup>+</sup>23, EK20b]. **fission** [LCP21, SCKH21]. **fitness** [ONA<sup>+</sup>20]. **fitted** [BSF20]. **Fitting** [ALA20, BK22, BK24, CQSG20, HGR<sup>+</sup>24, MFS22, MSS20, NSH23, TAC<sup>+</sup>23, ZZ23a]. **Five** [AD20, HGF20, LLJ<sup>+</sup>24, PLP<sup>+</sup>20]. **Five-Coordinate** [AD20]. **five-membered-heterocycle-embedded** [LLJ<sup>+</sup>24]. **five-site** [PLP<sup>+</sup>20]. **fixation** [JAP<sup>+</sup>24]. **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, AFR<sup>+</sup>24a]. **fluctuation** [SH23, XZW<sup>+</sup>21]. **fluid** [CM20a]. **fluids**

[SSYB<sup>+</sup>20]. **fluorescence** [AS21, LYX<sup>+</sup>22]. **fluorescent** [BVGB23, ZRSST20]. **Fluorine** [OE20]. **fluoro** [BAM<sup>+</sup>24]. **fluorophores** [FMK24]. **flupyradifurone** [BTL24]. **flux** [MNZGO<sup>+</sup>20]. **fly** [APP24, 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]. **Foldy** [IWN24]. **Following** [CG20, KdILC22, ETT21b]. **Force** [BAC20, LJ20, QB20, WSL<sup>+</sup>20, ALA<sup>+</sup>22, BJ22, BTL24, 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, KRW<sup>+</sup>24, KSP21, LCC<sup>+</sup>21]. **Form** [CWZD20]. **formally** [SSP23]. **formamide** [NHFS21]. **Formation** [GOY20, LZW<sup>+</sup>23, HL20, KPDB22, MDO<sup>+</sup>20, MLM<sup>+</sup>24, SSS<sup>+</sup>20a, dSSRVdM24, SKGG23, ZZ23b]. **formats** [VAP<sup>+</sup>21]. **formed** [SKT24]. **formic** [FP23]. **forms** [DSC20]. **formula** [Pan23]. **formulas** [IN23a]. **formulation** [CK22, Fed24]. **formulations** [SCvW22]. **foundation** [TSH<sup>+</sup>23]. **Four** [Yos24, DSB23, KWYN23]. **four-component** [KWYN23]. **Four-dimensional** [Yos24]. **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, Fed24, MSA<sup>+</sup>24, 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, GH23, 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, WdGG24, YBS<sup>+</sup>20, YIO20, ZQ24]. **Free-energy** [GBM20, KK23, SY21]. **frequencies** [OM23]. **frequency** [IN23a, SZL23]. **frequency-dependent** [IN23a, SZL23]. **friendly** [SKS21, ZK23]. **fromage** [RDS<sup>+</sup>20]. **Front** [AFR<sup>+</sup>24b, CGSP24b, HAC<sup>+</sup>23a, KWMPR24a, SNK24a, WTST24b, WLSC23b]. **frustrated** [FP22, MC24, 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,

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

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

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

[NSRK21]. **goal-oriented** [NSRK21]. **GoGreenGo** [PKT21]. **gold** [LL21a, NST<sup>+</sup>20, NSKN21, POPGS22]. **GPRI** [BA24]. **GPU** [ZKJ<sup>+</sup>23]. **GPU-specific** [ZKJ<sup>+</sup>23]. **gradient** [BMT<sup>+</sup>21, LC22, NG20, VV20b]. **gradients** [BSF20, VCL20]. **grafted** [Che23, GBM20]. **Grained** [MT20a, WSL<sup>+</sup>20, WZZ<sup>+</sup>20, BS23, CST23, GWN21, IL24, KGTL21, LL21b, LL22, MT19, SSDL<sup>+</sup>23]. **grand** [GGK20, ZKJ<sup>+</sup>23]. **grand-canonical** [GGK20]. **Graph** [CR24, BCN22, CdsB<sup>+</sup>21, NGD22, RSHG23, SKY24, WCY<sup>+</sup>24]. **Graph-based** [CR24, RSHG23]. **Graphene** [KK22c, BWS20, DZL<sup>+</sup>20, DOT22, RC22, SS23, SPT21, dSSCC24, 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]. **green** [AQIS<sup>+</sup>24]. **Gremlin** [CM20b]. **Gremlin-1** [CM20b]. **Grid** [Min20, CP23, RB24]. **grid-based** [CP23]. **GROMACS** [LKM20, MPP23]. **Ground** [Ari24, KWB24, Kop22b, BGPR24, 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, THH<sup>+</sup>24, TANC23, TT20, WCD<sup>+</sup>23, XSP<sup>+</sup>23, ZS22, ZHG<sup>+</sup>24, SMH21]. **Group-14** [LXP<sup>+</sup>22]. **group-CASPT2** [TT20]. **group-modified** [ZHG<sup>+</sup>24]. **groups** [CCZ23, HPG20]. **Growth** [XDZ23, BHR<sup>+</sup>21]. **GRP1** [PT20]. **guanidine** [RLHG<sup>+</sup>23]. **guanidine-quinoline** [RLHG<sup>+</sup>23]. **guanine** [XZX<sup>+</sup>22, BVGB23]. **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, CGSP24a, CBK<sup>+</sup>24]. **Gulari** [VFCG20].

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



[LLJ<sup>+</sup>24]. **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]. **hemoproteins** [FAK24]. **hepatitis** [MPuS<sup>+</sup>20]. **heptagons** [IW23]. **Herzberg** [Tou21]. **hetero** [GPM21b]. **hetero-bileptic** [GPM21b]. **heterobimetallic** [ZMH<sup>+</sup>21]. **heterocycle** [LLJ<sup>+</sup>24]. **heterocycles** [BSS<sup>+</sup>22]. **heterocyclic** [FP22, JGSA22]. **heterointerface** [SZP<sup>+</sup>20]. **heterojunction** [TANC23]. **Heterolytic** [LR20]. **heteronuclear** [KW22, SJZ<sup>+</sup>21]. **heteroporphyrins** [SaATR24]. **heterostructures** [PSM<sup>+</sup>20]. **Heusler** [SS24]. **hexa** [FDK22]. **hexa-** [FDK22]. **hexagonal** [NDK24]. **hexane** [NS22]. **Hf** [DBE20, AWK<sup>+</sup>23]. **Hg** [SSS<sup>+</sup>20a]. **hidden** [GM22, SSP23]. **Hierarchical** [NN20, dASRHB21, AÅFJ21, BTC24, LMPT21]. **High** [BLB20, EVKL21, KUNT20, LCP24, NBE<sup>+</sup>23, OKI<sup>+</sup>21, BSF20, DK23, GWN21, GVJ<sup>+</sup>22, IAF<sup>+</sup>24, KE23b, KWX23, KGG21, KDP<sup>+</sup>22, LHC<sup>+</sup>21, MZ21, PPV<sup>+</sup>21, RD23, XLW<sup>+</sup>22, ZWL24b]. **high-level** [BSF20]. **High-order** [EVKL21]. **High-performance** [BLB20]. **high-polarity** [DK23]. **high-resolution** [IAF<sup>+</sup>24]. **high-speed** [GWN21]. **High-throughput** [NBE<sup>+</sup>23]. **Higher** [HFPS20]. **highest** [KPHV23, LJW<sup>+</sup>23]. **highlight** [SNK24b]. **Highly** [JFZ<sup>+</sup>20, SHH<sup>+</sup>23b, SHH<sup>+</sup>23a]. **Hirshfeld** [LC22, MSE<sup>+</sup>21]. **histidine** [FAK24]. **histogram** [MT20b]. **HIV** [CBK<sup>+</sup>24, GG22, NPGP23, PWX<sup>+</sup>20, WCT<sup>+</sup>23]. **HIV-1** [CBK<sup>+</sup>24, 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, Che23, FV20, HMK23, HUO23, KGS<sup>+</sup>21, MN20, MKK<sup>+</sup>22, NG20, RPD<sup>+</sup>20a, RMBSPJSG24, 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]. **hydride** [GSSG24, MC24]. **Hydrides** [PWW20]. **Hydrido** [SLML24]. **hydroalkylation** [BXY<sup>+</sup>24]. **hydrocarbon** [NS22]. **hydrocarbons** [GAP21]. **Hydrocyanation** [JFZ<sup>+</sup>20]. **Hydrogen** [AKGD24, HS23, SKKG22, AV20, ARR22b, AD23, BCN22, CVGVN<sup>+</sup>20, ČNF23, CL23, CB20, DHN<sup>+</sup>21, DLH<sup>+</sup>23, GJL21, GH22b, KPTT21, KZ24,

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**  
 [JWS<sup>+</sup>24, PDP<sup>+</sup>24, ZLLL22]. **hydrophilicity** [MSA22a]. **hydrophobic**  
 [KPKS23]. **Hydrostatic** [SL20]. **hydroxychromones** [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]. **ICI** [PLT24]. **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]. **if** [RD24]. **IGMP** [LKK<sup>+</sup>23]. **II** [ABZ20b, AD20, GP21,  
 SVDS21, SSS<sup>+</sup>20a, WYC<sup>+</sup>24, YYS20, GH22a, KLC<sup>+</sup>24, KI24, RLHG<sup>+</sup>23].  
**II-Importance** [KLC<sup>+</sup>24]. **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]. **imaging** [Yos24]. **Imidazole** [CFOMCB<sup>+</sup>22, SKT24].  
**imidazopyridine** [ZOD<sup>+</sup>22]. **imino** [YFS20]. **immersive** [MSL<sup>+</sup>20].  
**Immunodeficiency** [KUNT20]. **Impact**  
 [MLM<sup>+</sup>24, KDKS21, OTZW24, OM23, SPSH20, VCRP23]. **impacts**  
 [MVV22]. **impedance** [KF24]. **Implementation**  
 [HAC<sup>+</sup>23b, NP23, PDP<sup>+</sup>24, YLZ<sup>+</sup>20, BPT<sup>+</sup>23, CSGVF<sup>+</sup>20, CPG21, FR21,  
 HGR<sup>+</sup>24, OMC<sup>+</sup>20, SSDL<sup>+</sup>23]. **implementations** [CHVF21]. **implications**  
 [KSP21]. **Implicit** [GRBN21, GCL<sup>+</sup>20, CCHS23, RPD<sup>+</sup>20a]. **Importance**  
 [HKS20, DSB23, KLC<sup>+</sup>24]. **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-silico** [dMBdAVdS24]. **in-situ** [MC24, WKG<sup>+</sup>23]. **inactivation**  
 [RPA<sup>+</sup>24]. **includes** [VWJ23]. **including** [FBP<sup>+</sup>22]. **inclusion** [YLZ<sup>+</sup>22].  
**Incorporating** [BTC24, Gie21]. **incorrectly** [GAP21]. **increase** [LKM20].  
**increases** [HREvdK<sup>+</sup>20]. **indenotetracene** [CCPR24]. **Independent**  
 [LC22, CSG<sup>+</sup>21, LGC21, WFBB22]. **index** [PC23, Sch22b]. **Indexes**  
 [WZZ<sup>+</sup>20, KdLLC22]. **indicator** [BA24]. **individual** [AD23, BRNB21].  
**INDO** [Gie21]. **INDO/S** [Gie21]. **Induced**  
 [QB20, CCPR24, EK20b, EK20c, FVSS20, KK22c, SCC<sup>+</sup>22, TTH<sup>+</sup>21a].  
**inexpensive** [Ben22]. **Influence**  
 [GAG20, MCP23, PT21, SGGG22, Brz22, CCHS23, SVDS21, SKT24].

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

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

**Information**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

**Interaction**

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

**Issue** [Ano20b, Ano20p, Ano20t, Ano20u, Ano20v, Ano20w, Ano20x, Ano20y, Ano20z, Ano20-27, Ano20-28, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20l, Ano20m, Ano20n, Ano20o, Ano20q, Ano20r, Ano20s, Ano20-29, Ano20-30, Ano20-55, Ano20-56, Ano20-57, Ano20-58, Ano20-59, Ano20-60, Ano20-31, Ano20-32, Ano20-33, Ano20-34, Ano20-35, Ano20-36, Ano20-37, Ano20-38, Ano20-39, Ano20-40, Ano20-41, Ano20-42, Ano20-43, Ano20-44, Ano20-45, Ano20-46, Ano20-47, Ano20-48, Ano20-49, Ano20-50, Ano20-51, Ano20-52, Ano20-53, Ano20-54, Ano21a, Ano21b, Ano21z, Ano21-27, Ano21-28, Ano21-29, Ano21-30, Ano21-31, Ano21-32, Ano21c, Ano21d, Ano21e, Ano21f, Ano21g, Ano21h, Ano21i, Ano21j, Ano21k, Ano21l, Ano21m, Ano21n, Ano21o, Ano21p, Ano21q, Ano21r, Ano21s, Ano21t]. **Issue** [Ano21u, Ano21v, Ano21w, Ano21x, Ano21y, Ano22a, Ano22b, Ano22-27, Ano22-28, Ano22-29, Ano22-30, Ano22-31, Ano22-32, Ano22c, Ano22d, Ano22e, Ano22f, Ano22g, Ano22h, Ano22i, Ano22j, Ano22k, Ano22l, Ano22m, Ano22n, Ano22o, Ano22p, Ano22q, Ano22r, Ano22s, Ano22t, Ano22u, Ano22v, Ano22w, Ano22x, Ano22y, Ano22z, Ano23a, Ano23b, Ano23-27, Ano23-28, Ano23-29, Ano23-30, Ano23-31, Ano23-32, Ano23c, Ano23d, Ano23e, Ano23f, Ano23g, Ano23h, Ano23i, Ano23j, Ano23k, Ano23l, Ano23m, Ano23n, Ano23o, Ano23p, Ano23q, Ano23r, Ano23s, Ano23t, Ano23u, Ano23v, Ano23w, Ano23x, Ano23y, Ano23z, Ano24b, Ano24c, Ano24d, Ano24e, Ano24f, Ano24g, Ano24h, Ano24i, Ano24j, Ano24k, Ano24l, Ano24m, Ano24n, Ano24o, Ano24p, Ano24q, Ano24r, Ano24s]. **Issue** [RPD<sup>+</sup>20b]. **iterative** [VV21]. **IV** [CMD<sup>+</sup>22, PPSP20, SVDS21].

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

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

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

[DGS24, WCY<sup>+</sup>24]. **Lantern** [LLKS23]. **Lantern-type** [LLKS23]. **lanthanides** [ALA<sup>+</sup>22, SLB23]. **Laplacian** [TTDT20]. **Large** [MFC20, NS22, UAC<sup>+</sup>23, AD23, AKGD24, BTC24, CJHW21, JKS23, KS21, KWX23, RBM<sup>+</sup>23, SSDL<sup>+</sup>23, UR23]. **large-scale** [BTC24, CJHW21]. **Large-Sized** [MFC20]. **laser** [LYX<sup>+</sup>22, LAM<sup>+</sup>23, MLX<sup>+</sup>24, SCC<sup>+</sup>22]. **laser-induced** [SCC<sup>+</sup>22]. **Late** [PWW20]. **LaTiO** [PGDD24]. **lattice** [NMF121]. **layer** [YrYqLhC23]. **layered** [EK20c]. **layers** [LMPT21]. **lead** [AQMM<sup>+</sup>23, dMBdAVdS24]. **lead-free** [AQMM<sup>+</sup>23]. **Leading** [AD20, NG20]. **leapfrog** [MIP<sup>+</sup>21]. **learned** [OTZW24]. **Learning** [LPP20, SKY24, BP22, CdSB<sup>+</sup>21, CBK<sup>+</sup>24, COK22, DGS24, HBT<sup>+</sup>20, HLV<sup>+</sup>24, JGK<sup>+</sup>22, KM22, KF24, KB22, KDP<sup>+</sup>22, LHB<sup>+</sup>24, MLC<sup>+</sup>23, MYYS24, NGD22, PSW<sup>+</sup>24, PDP<sup>+</sup>24, RDB23, RD24, SKL23, TXJT23, TCS<sup>+</sup>21a, VT24, WRBT21, WYC<sup>+</sup>24, WLSC23a, XZC<sup>+</sup>24, YFS20, Yos24]. **learning-assisted** [RD24, WRBT21]. **learning-guided** [CBK<sup>+</sup>24]. **length** [FR21, MVP<sup>+</sup>20]. **Lennard** [SG20]. **Lennard-Jones** [SG20]. **less** [CSWW20]. **leucine** [CGMRVBAI22]. **leucoindigo** [PPFL23]. **level** [ABNG22, BSF20, JK21, PHS<sup>+</sup>20]. **levels** [ERVN24, Kop22b]. **Lewis** [Brz23, FP22, HLV<sup>+</sup>24, MC24, NMMC21, OE20, PT21, PLZT23, ZS22]. **Li** [JX24, LEP<sup>+</sup>21, Ore24]. **Li-molecule** [Ore24]. **Libkrylov** [RBM<sup>+</sup>23]. **library** [JGK<sup>+</sup>22, KRSD<sup>+</sup>23, RBM<sup>+</sup>23, RDS<sup>+</sup>20, VAP<sup>+</sup>21, WHJM23]. **Lif** [VDK<sup>+</sup>20]. **lifetime** [FCB23]. **Ligand** [Ban20, JFZ<sup>+</sup>20, KW22, MXM20, NNT<sup>+</sup>20, AAe20, BTC24, BKM21, HGF20, IK21, KDLP21, KK23, KDP<sup>+</sup>22, LYKS23, MAKZ23, Ngo21, ÖLP<sup>+</sup>20, OM23, PMT<sup>+</sup>22, PNT<sup>+</sup>22, PSB<sup>+</sup>22, SNW22, TWT<sup>+</sup>22, TTK23, VWP<sup>+</sup>22, WCD<sup>+</sup>23, YIO20, ZOD<sup>+</sup>22]. **ligand-alkali** [OM23]. **ligand-based** [PMT<sup>+</sup>22]. **Ligand-Binding** [NNT<sup>+</sup>20, HGF20, Ngo21]. **ligand-free** [YIO20]. **ligand-ranking** [PNT<sup>+</sup>22]. **Ligand-stabilized** [KW22]. **Ligands** [Min20, SZLD20, DDSM23, GPM21b, LLKS23, RvWH23, SVDS21, TLS23]. **lignin** [BW22a]. **like** [DYG21, LSC<sup>+</sup>23, SAZ<sup>+</sup>23, YMSS23]. **limit** [CVGVN<sup>+</sup>20, SCKH21]. **limitations** [TZS<sup>+</sup>22]. **Limiting** [Cha24]. **limits** [WFBB22]. **LIMONADA** [CBB<sup>+</sup>21]. **linear** [OKK22, Sch22a, SNN<sup>+</sup>21, Tou21]. **linearized** [NSRK21]. **linearly** [BMA<sup>+</sup>24]. **link** [GH22a, KGTL21]. **linker** [GJL21]. **Links** [GFRNC21]. **LIO** [SDK20]. **Lipase** [VDK<sup>+</sup>20]. **lipid** [KFTB20b, WRBT21]. **lipids** [IL24, KCF<sup>+</sup>20]. **lipophilicity** [HS22]. **liquid** [CCZ23, IAS<sup>+</sup>24, KGS<sup>+</sup>22, LEP<sup>+</sup>21, MMF<sup>+</sup>24, SPSH20, ZWY<sup>+</sup>22]. **liquid-IAS<sup>+</sup>24**. **liquid-based** [LEP<sup>+</sup>21]. **Liquids** [VAL20, BUNO22b, Cer22, LWF<sup>+</sup>22, SI22, TPD21]. **lithium** [HM21, KE23b, Kop22b, Mil21, dSSCC24, SGT<sup>+</sup>20]. **lithium-based** [HM21]. **lithium-chloride** [Mil21]. **LLS** [GKO<sup>+</sup>22]. **LLS-SC** [GKO<sup>+</sup>22]. **load** [DLH<sup>+</sup>23]. **LOBSTER** [NEG<sup>+</sup>20]. **Local** [NEG<sup>+</sup>20, PKT21, SPT21, WSV20, BEKM24, DTA21, FB21, FDK22, FAK24, GFRNC21, HMK23, MAI22, PW20, TV22, VV20b]. **localization** [BMT23, LT23, WFLZ23]. **localized** [CdSB<sup>+</sup>21]. **locating**

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

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

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



**methotrexate-camptothecin** [PRH20]. **methoxyethyl** [MSA22a].  
**methoxyphenol** [KLC<sup>+</sup>24]. **methyl** [CCZ23, OAN<sup>+</sup>23, PGP<sup>+</sup>23, SKGG23].  
**methylene** [ERVN24]. **methylide** [SVTK<sup>+</sup>22]. **Metropolis** [EG20]. **Mg**  
 [SM22b, DSC20, GP21, JRS20, ZRSST20, ZDBZ20]. **MgCl** [AMM22]. **MgO**  
 [DA22]. **MH** [WTST24a]. **micellization** [ZK21]. **micro** [VHS<sup>+</sup>24].  
**micro-kinetic** [VHS<sup>+</sup>24]. **microhydrated** [GJL21]. **microkinetic**  
 [CJHW21, SC23]. **Microscale** [HZG<sup>+</sup>20]. **Microscopic** [PT20]. **microscopy**  
 [Yos24]. **Microsecond** [SSPK24]. **microsolvated** [OM22]. **microsolvation**  
 [STR20]. **MIDAS** [GJMPVR<sup>+</sup>20]. **midbond** [MEKH22]. **milder** [GM22].  
**mimetic** [HTFY21]. **minerals** [RCD<sup>+</sup>24]. **Minimal** [HHL<sup>+</sup>20, JGGPN21].  
**minimize** [AiIS<sup>+</sup>21]. **minimizing** [YBS<sup>+</sup>20]. **minimum**  
 [DC22a, RH21, SDH23]. **mismatch** [CR24]. **Mixed** [CDCT21, WTST24a].  
**Mixed-solvent** [CDCT21]. **mixture** [NS22]. **MkVsites** [LKM20]. **ML**  
 [TTK23]. **MLLPA** [WRBT21]. **MM** [ABNG22, BBC20, GH22a, LRqG<sup>+</sup>22,  
 LSCK23, Mar21, PCI23, SSS<sup>+</sup>20a, SHH<sup>+</sup>23b]. **MM-PBSA** [SHH<sup>+</sup>23b]. **Mn**  
 [TAB<sup>+</sup>24]. **MNDO** [FCB23]. **MNDO-MD** [FCB23]. **Mo** [MAM21].  
**Mo-Oxo** [MAM21]. **mobilities** [LHC<sup>+</sup>21]. **MoBioTools** [CLTMd<sup>+</sup>23].  
**MOCASSIN** [EG20]. **mode** [BEKM24, FDK22, FAK24, San21, SH23].  
**Model**  
 [GCL<sup>+</sup>20, HRT<sup>+</sup>20, LGM20, MT20a, SSS<sup>+</sup>20a, BW22a, BPDG21, BK24,  
 CC22, CX21b, CQSG20, DKB23, GSH23, Gie21, HKSW20, HPG20, IN23b,  
 IK21, IL24, KWYN23, KdILC22, KPKS23, LC22, MDO<sup>+</sup>20, MT19, MGCM21,  
 NGD22, PDL24, 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, WCY<sup>+</sup>24, WKL22, XAD20].  
**model-compounds** [BW22a]. **model/energy** [MGCM21]. **modeler**  
 [SKS21]. **Modeling** [AWID<sup>+</sup>20, BLP20, BS23, CMG<sup>+</sup>24, FVSS20, GNK<sup>+</sup>23,  
 KDLP21, KB22, LJ20, LWLC21, LDT<sup>+</sup>22, PAF<sup>+</sup>20, RCD<sup>+</sup>24, 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, NDK24,  
 PJJL23, PSG21, SSFS22b]. **models** [AVM21, BK22, BSR22, BP22,  
 CCHS23, CTBB20, DGS24, HPM<sup>+</sup>21, JGGPN21, KK23, KOD21, KTBS23,  
 LGJF22, LBH<sup>+</sup>22, LMPT21, MP24, MK22a, PLP<sup>+</sup>20, PSW<sup>+</sup>24, PMT<sup>+</sup>22,  
 PCI23, SKL23, SJA24, UB20, VHS<sup>+</sup>24, WP20]. **modes** [CBF<sup>+</sup>20, dBCdL20].  
**Modification** [AWID<sup>+</sup>20, Ban20]. **Modified**  
 [SG20, DOT22, XAD20, ZHG<sup>+</sup>24]. **Modifying** [PFPD21]. **modular**  
 [RBM<sup>+</sup>23]. **Modulation** [ZSD<sup>+</sup>20]. **module** [WRBT21, WLSC23a]. **MOF**  
 [ZHG<sup>+</sup>24, FP23]. **moiety** [KPTT21]. **Molecular**  
 [ARR22b, BR23, 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, AKGD24, AKN<sup>+</sup>20, AAL21,  
 AÅFJ21, AiIS<sup>+</sup>21, AR24, AS20, ALA<sup>+</sup>22, AMF<sup>+</sup>20, BUNO22b, BdLC21,  
 BRNB21, BAO<sup>+</sup>20, BSB<sup>+</sup>24, BTL24, BOPJ<sup>+</sup>21a, BP22, CFOMCB<sup>+</sup>22,  
 CLTMd<sup>+</sup>23, CDCT21, CX23, Che23, CSP20, CMD<sup>+</sup>22, CST23, DGS24,  
 DO20, DHN<sup>+</sup>21, DHD21, EVKL21, Fed22, Fed24, FDK22, FNY21, Gao20,

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

**molecular**

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

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

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

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

**molecules-in-molecules** [TSR21]. **Møller** [CSGVF<sup>+20</sup>, FKT21, Sán20].

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

[GNK<sup>+23</sup>]. **moments** [BSF20, LRKD23]. **Momentum** [FNY21, MR21].

**Mono** [ZXD20b, ZXD20a, HBM<sup>+20</sup>, MAKZ23]. **mono-** [MAKZ23].

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

[LHC<sup>+21</sup>, MMAZ<sup>+23</sup>]. **monomer** [ZLLL22]. **monooxygenase** [HYA<sup>+20</sup>].

**Monte** [DMD<sup>+21</sup>, EG20, GGK20, GNL<sup>+22</sup>, KCGK20, KEK23, PFSC20,

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

**MoO** [SM22b]. **moon** [HBM<sup>+20</sup>]. **MOPAC** [Gie21]. **MoSDeF** [DMD<sup>+21</sup>].

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

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

**MPCONF196** [PGH24]. **MPI** [AiIS<sup>+21</sup>, RB24]. **MPI-parallelization**

[RB24]. **MRCI** [ZRSST20]. **MSMS** [WK21]. **Mukaiyama** [LLS<sup>+22b</sup>].

**Multi** [HREvdK<sup>+20</sup>, AFR<sup>+24a</sup>, AS23, BBB<sup>+23</sup>, BMT<sup>+21</sup>, CMO<sup>+24</sup>,

PMT<sup>+22</sup>, SY21, VM23]. **multi-decker** [AS23]. **multi-descriptor**

[CMO<sup>+24</sup>]. **multi-parametric** [PMT<sup>+22</sup>]. **multi-purpose** [BMT<sup>+21</sup>].

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

[AFR<sup>+24a</sup>]. **multi-use** [BBB<sup>+23</sup>]. **multicanonical** [BAO<sup>+20</sup>].

**multiconfigurational** [HRTSS<sup>+20</sup>, TT20]. **multicore** [GJMPVR<sup>+20</sup>].

**multideterminant** [KRSD<sup>+23</sup>]. **multidimensional** [BCN22, GWN21].

**multifunctionalized** [AG21]. **multilayer** [IRB<sup>+23</sup>]. **multilevel** [SW21].

**Multilinear** [WSL<sup>+20</sup>]. **Multimolecular** [GP21]. **Multiple**

[SZLD20, MKK<sup>+22</sup>, POvG21, WCT<sup>+23</sup>, 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, UR23]. **Multiscale** [SSFS22b, FLT23, LGD<sup>+</sup>20, LGC21, Mar21]. **mussel** [MSA22a]. **mussel-inspired** [MSA22a]. **mutant** [BK22, CSP20]. **mutation** [SSPK24]. **mutations** [HB21, WCY<sup>+</sup>24]. **Mutual** [SKT24]. **Mycobacterium** [RDK<sup>+</sup>22].

**N** [ZHG<sup>+</sup>24, 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, KWB24]. **nanometer** [NAAP21]. **nanoparticle** [LBH<sup>+</sup>22]. **nanoparticles** [BA22, IL24]. **nanopores** [YC20]. **nanoreactor** [FP23]. **nanoribbons** [SPT21]. **nanoring** [YLZ<sup>+</sup>22]. **nanoscale** [SG20]. **nanoscopic** [CR24]. **NanoShaper** [WK21]. **nanostructures** [Che23]. **nanotube** [APS20, CTBB20]. **Nanotubes** [DBE20, BW22a, CBF<sup>+</sup>20, VCL20]. **Naphthalene** [NRH<sup>+</sup>20]. **naphthyridine** [WCD<sup>+</sup>23]. **naphthadithiophene** [BMA<sup>+</sup>24]. **naphthadithiophene-based** [BMA<sup>+</sup>24]. **Natural** [KL20, CB20, GRBN21, MH20, PW20, RPA<sup>+</sup>24, Sch22b, SD21]. **Nature** [MVP<sup>+</sup>20, PDC23, WG21, BRNB21, BPDG21, JX24, FDD<sup>+</sup>23, HSG21, Jab22b, KLC<sup>+</sup>24, 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, KRW<sup>+</sup>24, KOD21, MZ21, MLP22, NGD22, RTB23, SSM21, TIK21, WCY<sup>+</sup>24]. **networks** [SKY24, VFCG20]. **neural** [KRW<sup>+</sup>24, MZ21, MLP22, NGD22, SKY24, TIK21]. **neuraminidase** [SSPK24]. **neuroglobin** [FDK22]. **Neutral** [LL21a, BGS<sup>+</sup>20, KPKS23, MCP23, MP23]. **Neutralizing** [KUNT20]. **never** [SVR<sup>+</sup>24]. **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, BXY<sup>+</sup>24, MYYS24, PTP23, SS24, ZHG<sup>+</sup>24]. **Ni-catalyzed** [BXY<sup>+</sup>24]. **Ni-MOF-74** [ZHG<sup>+</sup>24]. **NIAS** [FPMD23]. **NIAS-Server** [FPMD23]. **nickel** [DSK21, LLKS23, ZZG<sup>+</sup>21]. **nickel-nickel** [LLKS23]. **nicotinic** [BRNB21]. **nitrate** [YC20]. **Nitreones** [PAS<sup>+</sup>20]. **nitride** [NDK24]. **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]. **nitrone** [BAM<sup>+</sup>24].  
**nitroprop** [SMB<sup>+</sup>23]. **nitrosyl** [KK23]. **nitrous** [KZJ21]. **nitroxide**  
 [MC23]. **NLi** [SKKG22]. **NMR** [Ben22, CMG<sup>+</sup>24, FBP<sup>+</sup>22, KWX23, LL22,  
 MPOC21, MPV22, MCD22, Sai23, TTDT20]. **NMR-data-assisted** [LL22].  
**NN** [LPP20]. **NO** [OKI<sup>+</sup>21]. **Noble** [YSMS24, APR21, MSYS23, YMSS23].  
**NOCV** [DGM22, GM22, GKA<sup>+</sup>23b, SBB<sup>+</sup>22, SM23]. **Noggin** [CM20b].  
**Non** [GAP21, KE23b, BdLC21, LGJF22, MP23, SKT24, TAC<sup>+</sup>23, VV21].  
**non-aqueous** [VV21]. **non-bonding** [MP23]. **non-classical** [BdLC21].  
**non-covalent** [SKT24]. **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, SJA24]. **noncovalent**  
 [BW22a, CSWW20, CTBB20, OE20, OM23, RMJ21, Sch22b, YW20].  
**nonelectrostatic** [VL22]. **nonequilibrium** [MPP23]. **nonfullerene**  
 [TANC23]. **Noniterative** [HFPS20]. **Nonlinear**  
 [BSR22, RMBSPJSG24, 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, VT24, LHC<sup>+</sup>21, PPP21, RDK<sup>+</sup>22, RD24, 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** [BVGB23, CTBB20]. **nucleophilic** [CRT<sup>+</sup>21]. **nucleotide**  
 [XZX<sup>+</sup>22]. **Nudged** [MA23b, MA23a, ZLLL22]. **Number** [VHS<sup>+</sup>24, 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, IAF<sup>+</sup>24, KPTT21,  
 MC23, MCP23, MBBU23, SGSB23, SWF<sup>+</sup>20, SWM<sup>+</sup>20b, SVTK<sup>+</sup>22, TYZ20].  
**O-compounds** [MCP23]. **O-H** [KPTT21]. **Obelin** [GOY20]. **obtain**  
 [dMBdAVdS24, FNY21]. **obtained** [UKBD23]. **OC** [HS23]. **occupation**  
 [ASW20, Sch22a, SD21]. **occupied** [KPHV23]. **OCOH** [dCVARN20].  
**octahedra** [PGDD24, PDL24]. **octamer** [Bal20b]. **octanol** [SHH<sup>+</sup>23b].  
**OCTMCCO** [LZW<sup>+</sup>23]. **O =** [ARR22b]. **off** [LK22]. **off-center** [LK22].  
**offs** [WKL22]. **OLEDs** [ZWL24b]. **oligonucleotides** [KZOV23]. **Omicron**  
 [KLZ<sup>+</sup>23]. **on-surface** [LHG<sup>+</sup>23]. **On-the-fly** [APP24, OSHT20, RBM<sup>+</sup>23].  
**one** [BBC<sup>+</sup>21a, SNK24b, WKG<sup>+</sup>23]. **one-electron** [BBC<sup>+</sup>21a]. **one-photon**  
 [SNK24b]. **one-step** [WKG<sup>+</sup>23]. **ONIOM** [KWX23]. **online** [WRVP22].  
**onto** [AWK<sup>+</sup>23]. **OO** [SVTK<sup>+</sup>22]. **Open**  
 [SM23, AAID22, FR21, HAC<sup>+</sup>23b, IW24, MNBG<sup>+</sup>21, PSGL21, RBM<sup>+</sup>23].  
**open-shell** [IW24]. **open-source**  
 [AAID22, FR21, HAC<sup>+</sup>23b, MNBG<sup>+</sup>21, PSGL21, RBM<sup>+</sup>23]. **Opening**  
 [VDK<sup>+</sup>20]. **OpenMM** [BPT<sup>+</sup>23]. **operators** [BBC<sup>+</sup>21a, CTPJH22]. **OPLS**  
 [ZWY<sup>+</sup>22]. **OPLS-AA** [ZWY<sup>+</sup>22]. **oppositely** [HPG20]. **optical**

[AQRA<sup>+</sup>23, BA22, BSR22, JS21, JMV21, LM24, LRKD23, PSA<sup>+</sup>23, RMBSPJSG24, STB<sup>+</sup>20, TAB<sup>+</sup>24, 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, LSCK23, MMK<sup>+</sup>20]. **Optimized** [GH22a]. **optimizing** [RDB23]. **Opto** [AQIS<sup>+</sup>24, BMA<sup>+</sup>24]. **Opto-electronic** [AQIS<sup>+</sup>24, BMA<sup>+</sup>24]. **Optoelectronic** [dCB23, 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, Fed24, GRBN21, HTTT23, HCS<sup>+</sup>20, KK23, KPHV23, MSA<sup>+</sup>24, NAN<sup>+</sup>23, NEG<sup>+</sup>20, PDL24, PW20, Sch22b, SD21, TWT<sup>+</sup>22, TSH<sup>+</sup>23, VKSS24]. **orbital-based** [TWT<sup>+</sup>22]. **orbitals** [BTSB22, FV20, KL20, MH20]. **order** [CSGVF<sup>+</sup>20, DTA21, EVKL21, FKT21, FYIO23, GX20, HD21, QLW<sup>+</sup>22b, Sán20, YW20]. **ordering** [PDL24]. **Organic** [LPP20, AFR<sup>+</sup>24a, AZKM22, CCZ23, FB20, GGK20, HRTSS<sup>+</sup>20, KGS<sup>+</sup>21, KS21, KPHV23, LPF<sup>+</sup>23, LCP24, 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]. **organo** [SKY24]. **organo-transition** [SKY24]. **organocatalysts** [FP22]. **organophosphorus** [AR24, PDP<sup>+</sup>24, 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, BXY<sup>+</sup>24, TANC23]. **ortho** [VM23]. **ortho-nitrobenzaldehyde** [VM23]. **orthogonal** [CB20]. **oscillators** [BS23]. **Other** [FMFG20, TAC<sup>+</sup>23]. **outcome** [DGS24]. **overlap** [BK24, 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, RCD<sup>+</sup>24, SGRN24, 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, KZ24, NAAP21, SGRN24, SaATR24, WW24]. **oxygen** [SaATR24]. **oxygen-centered** [KZ24]. **oxygen-oxygen** [HL20]. **oxygen-preadsorbed** [WW24]. **oxynitride** [HM21].

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

BBK<sup>+21</sup>, CP23, GVJ<sup>+22</sup>, JKK<sup>+21</sup>, JKS23, SSDL<sup>+23</sup>, WMZJ20, YWGY22].  
**parallelization** [NN20, RB24, YLZ<sup>+20</sup>]. **parallelized** [AiIS<sup>+21</sup>].  
**paramagnetism** [GSSG24]. **parameter** [POPGS22, RB22].  
**parameterization** [OC23]. **Parameterizing** [KOD21]. **parameters**  
 [BTL24, BK24, DTA21, GH22a, KDLP21, LKM20, LBH<sup>+22</sup>, MH22, PNT<sup>+22</sup>].  
**parametric** [PMT<sup>+22</sup>]. **parametrization** [GKO<sup>+22</sup>, KYM20]. **part**  
 [MR21, MPR22, RLHG<sup>+23</sup>]. **partial** [LK22, MM24]. **particle**  
 [CN21, WKD<sup>+21</sup>]. **particle-field** [WKD<sup>+21</sup>]. **particles** [LSC<sup>+23</sup>].  
**partition** [AYO20, CSGVF<sup>+20</sup>, LC22, SHH<sup>+23b</sup>]. **Partitions** [TLD<sup>+22</sup>].  
**Parzen** [AZKM22]. **PASSerRank** [TXJT23]. **Path**  
 [SZLD20, Shi22, AKR21, GSD<sup>+22</sup>, RH21, TAB<sup>+24</sup>]. **paths**  
 [ETT21b, MA23b, SDH23]. **pathway** [DSB23, HL20, PPRS22, XZC<sup>+24</sup>].  
**pathways** [AST24, BBC20, CG20, DWSX20]. **pattern** [XDZ23]. **patterns**  
 [HS22, KLZ<sup>+23</sup>]. **Pb** [LXP<sup>+22</sup>, WTST24a]. **PbI** [XZW<sup>+21</sup>]. **PBSA**  
 [SHH<sup>+23b</sup>, SHH<sup>+23a</sup>]. **PCM** [CC22]. **Pd** [ABZ20b, PTP23, SS24].  
**Pd-PEPPSI** [ABZ20b]. **PDB** [RB22]. **PDB-to-parameter** [RB22]. **PdBe**  
 [Tze21]. **PEACH** [ZK21]. **PEB8** [BR23]. **PEC4** [BR23]. **PEC8** [BR23].  
**penicillin** [CD20]. **pentacoordinate** [FDK22]. **pentaerythritol** [BR23].  
**pentahalides** [PT21]. **Pep** [SKS21]. **PepPro** [XZ20]. **PEPPSI** [ABZ20b].  
**peptidase** [CD20]. **Peptide**  
 [XZ20, EIT<sup>+21</sup>, GG22, KZOV23, SKS21, SSS<sup>+20b</sup>, UAC<sup>+23</sup>].  
**peptide-based** [KZOV23]. **Peptide-Protein** [XZ20]. **peptides** [PRIP24].  
**per-** [MHA<sup>+23</sup>]. **perfluorinated** [FDD<sup>+23</sup>]. **perfluoroalkyl** [MVV22].  
**perform** [CKH23, MY24]. **Performance**  
 [BBK20, GSH23, NRH<sup>+20</sup>, PB20, BLB20, LKM20, MH22, MKK<sup>+22</sup>,  
 OKI<sup>+21</sup>, SFS24, dASRHB21, SS24, TTK23]. **performed** [MAM21].  
**Performing** [Zac20, FYIO23]. **period** [LB21, LB22]. **Periodic**  
 [SDK20, HAC<sup>+23b</sup>, PKT21, PSMPB21, SZP<sup>+20</sup>, YAO20]. **Periselectivity**  
 [SHH<sup>+24</sup>]. **permeability** [ZSD<sup>+20</sup>]. **permutation** [FYIO23].  
**Permutationally** [OKK22]. **perovskite**  
 [AQRA<sup>+23</sup>, LM24, SZP<sup>+20</sup>, XZW<sup>+21</sup>]. **perovskites**  
 [AQMM<sup>+23</sup>, ABAQ<sup>+23</sup>, KGS<sup>+21</sup>, PGDD24, PDL24, dARW<sup>+23</sup>]. **peroxide**  
 [CL23, DHN<sup>+21</sup>]. **peroxides** [MC23, WKG<sup>+23</sup>]. **peroxy** [WKG<sup>+23</sup>].  
**persistent** [BPDG21]. **perspective**  
 [AVM21, BBL<sup>+22</sup>, DF22, LKAT22, LT23, NI22, PPSP20, SWM<sup>+20b</sup>, SCC<sup>+22</sup>].  
**persulfate** [ARA22]. **Perturbation**  
 [NNT<sup>+20</sup>, AAe20, FKT21, GX20, MH20, NTK21, OE20, Sán20, YBS<sup>+20</sup>].  
**perturbations** [PKT21]. **perturbed** [PDGD23]. **pesticide** [BTL24]. **PFAS**  
 [MPV22]. **Pfizer** [GLC<sup>+22</sup>]. **PH** [PT20, CR24, SSS<sup>+20a</sup>, WdGG24].  
**pH-consistent** [CR24]. **pharma** [IRB<sup>+23</sup>]. **pharmacophore**  
 [KDP<sup>+22</sup>, MLG<sup>+21b</sup>]. **pharmacophore-based** [MLG<sup>+21b</sup>]. **PharmRF**  
 [KDP<sup>+22</sup>]. **Phase**  
 [HFPS20, VFCG20, AZKM22, BPT<sup>+23</sup>, CM20a, DC22b, EK20c, IMT<sup>+21</sup>,  
 LWF<sup>+22</sup>, OM23, SW21, SGSB23, SNK24b, 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]. **phonon** [SS24].  
**Phonons** [DBE20]. **phosphate** [DPSG20, HUUO23, SGRN24, SGGG22].  
**phosphine** [SGRN24]. **phosphorane** [STB<sup>+</sup>20]. **phosphocholine** [ZK21].  
**phosphodiester** [GP21]. **phosphoglucose** [DPSG20]. **phosphorescent**  
 [WYC<sup>+</sup>24]. **phosphorus** [ASL<sup>+</sup>20, HM21]. **phosphorus-based** [ZS22].  
**phosphoryl** [SGRN24]. **photo** [CCPR24, KFTB20b]. **photo-induced**  
 [CCPR24]. **photo-switchable** [KFTB20b]. **photoacidity** [GSH23].  
**Photocatalytic** [BWS20]. **photochemical** [CG20]. **Photochemistry**  
 [FCPG20]. **Photodissociation** [dSSRVdM24]. **photodynamic**  
 [ASL<sup>+</sup>20, DART21, RPA<sup>+</sup>24, DMTR22]. **photoionization** [AAL21].  
**Photoisomerization** [YXGZ20]. **photon** [SNK24b]. **photooxidation**  
 [KDKS21]. **Photophysical** [DART21, WYC<sup>+</sup>24]. **Photophysics** [BVGB23].  
**photoproperties** [TANC23]. **Photoprotein** [GOY20]. **photoresponsive**  
 [YLZ<sup>+</sup>22]. **photosensitizers** [ASL<sup>+</sup>20, DART21, RPA<sup>+</sup>24].  
**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, SSPK24]. **platform** [BBB<sup>+</sup>23, CSG<sup>+</sup>21, PSGL21, ZK23].  
**platform-independent** [CSG<sup>+</sup>21]. **platinum**  
 [HBM<sup>+</sup>20, NAAP21, WYC<sup>+</sup>24]. **play** [FM21, KE23b]. **Plesset**  
 [FKT21, CSGVF<sup>+</sup>20, Sán20]. **plugin** [EK20a]. **PMe** [PTP23]. **pnicogen**  
 [KS24]. **Pnictogen** [AR24]. **pockets** [XZX<sup>+</sup>22]. **Point**  
 [MXM20, BSF20, CST23, MH22, PP23, PKT21, TTK23]. **points** [DTA21].  
**Poisson**  
 [BSB<sup>+</sup>24, CX21b, NSRK21, RCC21, SCvW22, UYJ<sup>+</sup>24, 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].  
**polyacenes** [MG24]. **polyacethylene** [BSR22]. **polyalcohol** [KSRB<sup>+</sup>21].  
**polyatomic** [SSO<sup>+</sup>20]. **polyazaheterocycle** [MIP<sup>+</sup>22]. **polybase** [HLV<sup>+</sup>24].  
**polychromism** [RCD<sup>+</sup>24]. **polycyclic** [GAP21]. **polydiacetylene** [NLC23].  
**polyenes** [FCB23]. **Polyethyleneimine** [BAC20, MT21, TPB22].  
**Polyethylenimine** [MT20a, MT19]. **polyfluoroalkyl** [MHA<sup>+</sup>23]. **polymer**

[AFR<sup>+</sup>24a, Che23, WKD<sup>+</sup>21]. **polymer-grafted** [Che23]. **polymeric** [AÄFJ21]. **polymerization** [ARA22, MLB<sup>+</sup>23, MYYS24, 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** [BA24, 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, CBK<sup>+</sup>24, ZOD<sup>+</sup>22]. **Potential** [KFTB20b, PCB<sup>+</sup>24, APP24, AS20, BBC<sup>+</sup>21a, ERVN24, EK20a, GFRNC21, GP21, HS23, HPM<sup>+</sup>21, KRW<sup>+</sup>24, KM22, KSRB<sup>+</sup>21, Kop22b, KS24, KGD<sup>+</sup>21, MSL<sup>+</sup>20, MK22b, OKI<sup>+</sup>21, PPRS22, RKC21, SDK20, Sts20, SSO<sup>+</sup>20, THH<sup>+</sup>24, Tik23, WTST24a, WRVP22, XLW<sup>+</sup>22, XZC<sup>+</sup>24, YFH<sup>+</sup>21, ZZ23a]. **potential-energy** [MSL<sup>+</sup>20]. **potentials** [BSS<sup>+</sup>22, BBC<sup>+</sup>21a, Cha24, GWN21, LT23, MLB<sup>+</sup>23, MAM<sup>+</sup>23, MLP22, PSW<sup>+</sup>24, RLHG<sup>+</sup>23, SM22b, SG20, TTK23, ZFRM20]. **ppdx** [COK22]. **Pr** [SLML24]. **preadsorbed** [WW24]. **precatalyst** [ABZ20b]. **precision** [XLW<sup>+</sup>22]. **precomputed** [BTC24]. **preconditioning** [RH21]. **precursor** [BVC<sup>+</sup>23]. **precursors** [GM22]. **predefined** [BBSFA22]. **predict** [BA24, Ben22, PDP<sup>+</sup>24]. **predictability** [NGD22]. **Predicted** [CLS<sup>+</sup>20, LWF<sup>+</sup>22]. **Predicting** [APS20, BF22, DRBT24, HBT<sup>+</sup>20, KLC<sup>+</sup>24, MYYS24, QLW<sup>+</sup>22b, WCY<sup>+</sup>24, HLV<sup>+</sup>24, 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, TXJT23, YFS20, ABZ20b, AAe20, AS23, DPY<sup>+</sup>22, Dor20, GSSG24, 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** [WYC<sup>+</sup>24, DGS24, WCT<sup>+</sup>23]. **predictive** [FB20]. **prefer** [APS20]. **preference** [PFPD21]. **preferences** [DA22]. **Preliminary** [GP21, ZLLL22]. **preparation** [CR24, 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]. **principle** [LM24]. **Principles** [DBE20, AWK<sup>+</sup>23, BRNB21, DLH<sup>+</sup>23, EK20b, EPT21, KDKS21, KPKS23, PM21, SS24]. **principles-based** [PM21]. **PrNCN** [SLML24]. **PrNCO** [SLML24]. **Probability** [TLD<sup>+</sup>22, RD23]. **probe** [KTBS23, NP23]. **Probing** [GH22a, WG20, Tou21]. **problem** [DWSX20, LBH<sup>+</sup>22]. **problems** [MA23b]. **procedure** [AFR<sup>+</sup>24a]. **Process** [WLZM20, BP22, KK23, MP24, 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**



[AKGD24, BK24, Che23, 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, GH23]. **proline** [HB21]. **promenades** [MSL<sup>+</sup>20]. **Promising** [CP23, TAB<sup>+</sup>24]. **promoted** [OSM20]. **promotion** [MGCM21]. **propene** [BR23, DRBT24, 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, BMA<sup>+</sup>24, BSR22, BTSB22, CCZ23, CdSB<sup>+</sup>21, CM20a, CSG<sup>+</sup>21, CA22, DART21, DYGM21, HMK23, HD21, IW23, JS21, JMV21, KPPT21, KBHG23, LM24, LRF<sup>+</sup>21, LWF<sup>+</sup>22, LRKD23, LXP<sup>+</sup>22, LDT<sup>+</sup>22, dCB23, MMAZ<sup>+</sup>23, MCD22, NPGP23, OAN<sup>+</sup>23, PCB<sup>+</sup>24, PSM<sup>+</sup>20, PDP<sup>+</sup>24, PCI23, PSA<sup>+</sup>23, RMS<sup>+</sup>23, RMBSPJSG24, SBFSJMLU23, SGT<sup>+</sup>20, STB<sup>+</sup>20, VV20b, WSV20, WMJ<sup>+</sup>22, WYC<sup>+</sup>24, XDZ23, ZWL<sup>+</sup>24a]. **Property** [GZFSM21, DGS24]. **Property-oriented** [GZFSM21]. **propranolol** [IAS<sup>+</sup>24]. **propylene** [AMM22]. **protease** [BVC<sup>+</sup>23, dSCCN21, PWX<sup>+</sup>20, PPP21, UAC<sup>+</sup>23, YC23]. **proteases** [dMBdAVdS24, CBK<sup>+</sup>24]. **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, PJJL23, QLW<sup>+</sup>22b, RDK<sup>+</sup>22, San21, SKL23, SY21, SEZ20, SLMA21, SNW22, WCY<sup>+</sup>24, WGKG20, YIO20, ENR<sup>+</sup>24]. **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]. **Protein3D** [ENR<sup>+</sup>24]. **Proteins** [HHL<sup>+</sup>20, LJ20, BPDG21, CGSP24a, 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, LSC24, MPP23, MPV22, VWP<sup>+</sup>22]. **protocols** [PDP<sup>+</sup>24]. **Proton** [MFC20, AIV20, BBC20, BBBP<sup>+</sup>23, ĆNF23, DC22b, Nan24, RCC<sup>+</sup>20, SW21]. **proton-coupled** [ĆNF23]. **Protonated** [BAC20, MT21, ZHHS21]. **protonation** [CR24]. **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, SS24, SVDS21, SSM21]. **pucker** [KB22]. **pull** [ARR22a, GPM21b, KdILC22]. **pulse** [LAM<sup>+</sup>23]. **pulses** [MLX<sup>+</sup>24]. **pump** [CGSP24a]. **pure** [BUNO22b, WTST24a, WMJ<sup>+</sup>22]. **purpose**

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

**Q** [SK20, ZDBZ20, XZC<sup>+24</sup>]. **Q-learning** [XZC<sup>+24</sup>]. **Qball** [AME<sup>+21</sup>]. **QC** [KGD<sup>+21</sup>]. **QIDH** [RMBSPJSG24]. **QM** [Mar21, ABNG22, BBC20, GH22a, LRqG<sup>+22</sup>, LSCK23, Mar21, PWW20, PCI23, SSS<sup>+20a</sup>]. **QM/MM** [ABNG22, BBC20, GH22a, LRqG<sup>+22</sup>, LSCK23, Mar21, PCI23, SSS<sup>+20a</sup>]. **QM/QM** [PWW20]. **QM7b** [VT24]. **QM9** [VT24]. **QMCube** [Mar21]. **QSAR** [BHR<sup>+21</sup>, DF22, SS20]. **QSAR/MD** [HKFT21]. **QSARINS** [CSG<sup>+21</sup>]. **QSARINS-Chem** [CSG<sup>+21</sup>]. **QTAIM** [AMF<sup>+20</sup>]. **quadrature** [IN23a]. **Quadruple** [Tze21, PTP23]. **Qualitatively** [Sts20]. **Quality** [RD23, AVM21, FB20, LB21, LB22, MK22a, SLB23]. **Quantification** [AWK<sup>+23</sup>]. **quantify** [LKK<sup>+23</sup>, Sch22b]. **quantifying** [IBL20]. **Quantitative** [AV20, BGS<sup>+20</sup>]. **quantity** [RD23]. **quantized** [VCRP23]. **Quantum** [AWID<sup>+20</sup>, IRB<sup>+23</sup>, MMF<sup>+24</sup>, Ooy20, PAS<sup>+20</sup>, PHS<sup>+20</sup>, Pil20, PSA<sup>+23</sup>, SR23, AKGD24, AA20, BS23, BRNB21, BHR<sup>+21</sup>, BBK<sup>+21</sup>, CLTmd<sup>+23</sup>, CSGVF<sup>+20</sup>, CP23, FDK22, GPEK<sup>+20</sup>, GP21, HKS20, HUuo23, HBT<sup>+20</sup>, JCMHT22, JGGPN21, KRSD<sup>+23</sup>, KFLP21, KB22, LGM20, LGM22, LYX<sup>+22</sup>, LCLB24, MLC<sup>+23</sup>, OKI<sup>+21</sup>, OE20, Pwx<sup>+20</sup>, PGP<sup>+21</sup>, RDB23, SPSH20, SSMP23, SIW21, SYS<sup>+21</sup>, SC23, SNN<sup>+21</sup>, Shi22, SKT24, dSSCC24, SCC<sup>+22</sup>, TPD21, TCS<sup>+21a</sup>, VT24, VWJ23, XSP<sup>+23</sup>]. **quantum-chemical** [BHR<sup>+21</sup>, SKT24, SCC<sup>+22</sup>, VWJ23]. **quantum-classical** [HUuo23]. **quantum-dot** [LCLB24]. **quasi** [Cer22, NSKN21]. **quasi-degenerate** [NSKN21]. **quasi-harmonic** [Cer22]. **quaternary** [ODL20]. **quaterthiophene** [CBF<sup>+20</sup>]. **QuBiLS** [GJMPVR<sup>+20</sup>]. **QuBiLS-MIDAS** [GJMPVR<sup>+20</sup>]. **quest** [MMAZ<sup>+23</sup>]. **quick** [Vyb23]. **quinoline** [RLHG<sup>+23</sup>].

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

[CV22, GPEK<sup>+</sup>20, MH20, OAN<sup>+</sup>23, PGP<sup>+</sup>21]. **Random**  
 [HFPS20, VF20, YW20]. **Range** [BBK20, AS21, CHVF21, GH22a,  
 GAP21, HTTT23, HTFY21, HCS<sup>+</sup>20, RMBSPJSG24]. **range-separated**  
 [RMBSPJSG24]. **rank** [TXJT23]. **ranking** [PNT<sup>+</sup>22]. **Raphson** [MT20b].  
**Raphson/singular** [MT20b]. **rapid** [LLZ<sup>+</sup>23, MT20b]. **rare**  
 [RLR<sup>+</sup>20, RD23, VZG<sup>+</sup>24, ZWL<sup>+</sup>24a]. **Ras** [MM20]. **Rashba** [dARW<sup>+</sup>23].  
**rate** [dCVARN20]. **rates** [CGMRVBAI22, GK24, KWMPR24b]. **Rational**  
 [DSK21, SHP<sup>+</sup>23, ZZG<sup>+</sup>21, BXY<sup>+</sup>24, ZBH<sup>+</sup>23]. **ray** [EK20a, FB20]. **Rb**  
 [SL20, AQMM<sup>+</sup>23, AQIS<sup>+</sup>24, RNP20]. **RBD** [KLZ<sup>+</sup>23]. **RC**  $\equiv$  [WLZM20].  
**RDFE** [MPP23]. **R**  $\equiv$  [WLZM20]. **Reaction**  
 [QB20, SLR<sup>+</sup>20, AMM22, BBY<sup>+</sup>21, BBC20, BCN22, CG20, CS20, CD20,  
 CRT<sup>+</sup>21, DGS24, DWSX20, DPY<sup>+</sup>22, DLH<sup>+</sup>23, GSD<sup>+</sup>22, HL20,  
 HREvdK<sup>+</sup>20, LLS<sup>+</sup>22b, LRqG<sup>+</sup>22, LBH<sup>+</sup>22, MNZGO<sup>+</sup>20, MIP<sup>+</sup>22,  
 MNBG<sup>+</sup>21, MA23b, NAAP21, PRF20, PDP<sup>+</sup>24, PM21, SYS<sup>+</sup>21, SSS<sup>+</sup>20a,  
 SKGG23, SSM21, SCZ<sup>+</sup>21, TYZ20, XZC<sup>+</sup>24, YGG<sup>+</sup>23, ZLLL22, ZS22].  
**Reactions** [ĆNF23, OOY20, SK20, ABZ20b, BAM<sup>+</sup>24, BBBP<sup>+</sup>23, GCP22,  
 LSC24, LHG<sup>+</sup>23, MH22, MDO<sup>+</sup>20, MN20, PRF20, RCC<sup>+</sup>20, SKY24,  
 SYS<sup>+</sup>21, SC23, SMB<sup>+</sup>23, SSYB<sup>+</sup>20, WKCP21, dCVARN20]. **Reactive**  
 [TSH<sup>+</sup>23, BJ22, FVSS20, PSW<sup>+</sup>24, ZG21]. **Reactivities** [MML<sup>+</sup>23].  
**Reactivity** [SHM<sup>+</sup>20, VAL20, BA24, CMD<sup>+</sup>22, GM22, KFLP21, KTBS23,  
 LGJF22, LMPT21, MAI22, ZS22]. **reading** [VAP<sup>+</sup>21]. **reagents** [SCZ<sup>+</sup>21].  
**Real** [MSS20, CCPR24, GCP22, HAC<sup>+</sup>23b, KdILC22]. **Real-time**  
 [MSS20, CCPR24, HAC<sup>+</sup>23b]. **Realistic** [IN23b, ZWY<sup>+</sup>22]. **reality**  
 [MSL<sup>+</sup>20]. **Realization** [SH23]. **Rearrangement** [PGP<sup>+</sup>23]. **reason**  
 [RTB23]. **Reasoning** [QB20]. **ReaxFF** [WW24]. **Receptor**  
 [BWM20, BRNB21, BHR<sup>+</sup>21, CSP20, TPZ<sup>+</sup>20, TZS<sup>+</sup>22, VWP<sup>+</sup>22, WGKG20].  
**receptor-** [CSP20]. **receptor-flexible** [VWP<sup>+</sup>22]. **Receptor-Membrane**  
 [BWM20]. **Receptors** [Min20]. **recognition**  
 [BPL<sup>+</sup>22, BRNB21, DSPG20, KGD<sup>+</sup>21, SCCZ21, WCT<sup>+</sup>23]. **Recognizing**  
 [HGF20]. **recombination** [KWMPR24b]. **reconstruction**  
 [ABTM22, PPV<sup>+</sup>21]. **reconstructions** [OAC23]. **Record** [HZG<sup>+</sup>20].  
**Recovering** [RGGD21]. **recovery** [DK23]. **rectangular** [AYO20].  
**recurrence** [Gao20, IN23a]. **recurrence-relation** [Gao20]. **recurrent**  
 [TIK21]. **Redox** [RvWH23, AFR<sup>+</sup>24a, Cha24, MLB<sup>+</sup>23, RLHG<sup>+</sup>23, SM22b].  
**Redox-active** [RvWH23]. **reduced** [Ore24]. **reductase** [CFOMCB<sup>+</sup>22].  
**Reduction** [ABZ20b, AR20, MC24, NAAP21, PPSP20]. **reference**  
 [BTSB22, KWYN23, VM23, WKL22]. **references** [LWC<sup>+</sup>24]. **Refined**  
 [KSRB<sup>+</sup>21]. **refinement** [NSRK21, RCC21]. **regime** [FCPG20]. **regio**  
 [BXY<sup>+</sup>24, SMB<sup>+</sup>23]. **regio-** [BXY<sup>+</sup>24, SMB<sup>+</sup>23]. **region** [FKT21]. **regions**  
 [HTTT23, SSPK24]. **Regioselective** [JFZ<sup>+</sup>20]. **Regioselectivity** [JFZ<sup>+</sup>20].  
**regression** [BP22, MP24, OKK22, SS23]. **regularized** [SS23]. **regulating**  
 [PPRS22, WSV20]. **regulator** [CDCT21]. **Reinforcement**  
 [LHB<sup>+</sup>24, JGK<sup>+</sup>22]. **related** [BPL<sup>+</sup>22, CdSB<sup>+</sup>21, MLB<sup>+</sup>23]. **relation**  
 [Gao20]. **relationship** [HS22]. **relationships** [MML<sup>+</sup>23]. **relative**

[MPP23, PWX<sup>+20</sup>, ZQ24]. **Relativistic** [GH22b, GH23, IWN24, 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, LWC<sup>+24</sup>]. **reliably** [APP24]. **REMD** [MGB<sup>+22</sup>]. **removal** [FNY21]. **renewable** [LM24]. **renormalization** [BBK<sup>+21</sup>, TT20, XSP<sup>+23</sup>]. **repair** [CGMRVBAl22]. **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, WCY<sup>+24</sup>]. **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, SSPK24]. **resolution** [IAF<sup>+24</sup>, LSP23]. **resolved** [AS21, ABNG22, CS23, KRW<sup>+24</sup>]. **Resolving** [WdGG24, XCJ20]. **Resonance** [OAN<sup>+23</sup>, WG21, AV20, ARR22b, ERVN24, LL21b, NHFS21, Wan21a, Wan21b]. **resonance-assisted** [AV20, ARR22b]. **resonances** [BBY<sup>+21</sup>]. **resource** [LGD<sup>+20</sup>]. **respect** [CC22]. **Response** [MLX<sup>+24</sup>, Wan21a, CC22, KZ24, Tou21]. **responsive** [KCF<sup>+20</sup>]. **Restoring** [WKD<sup>+21</sup>]. **restrained** [QLC<sup>+20</sup>]. **restrained-ensemble** [QLC<sup>+20</sup>]. **Restraints** [MXM20]. **Results** [BdLC21, Sts20]. **retinal** [GK24]. **revealed** [LHG<sup>+23</sup>]. **revealing** [ARR22b, HTTT23]. **reveals** [BPDG21, HREvdK<sup>+20</sup>, JRS20, MAM21, ONA<sup>+20</sup>, SSPK24]. **Review** [ZFRM20]. **revisited** [NSH23, PC23, SWF<sup>+20</sup>, TTT<sup>+21</sup>]. **Revisiting** [MMAZ<sup>+23</sup>, SCZ<sup>+21</sup>]. **RhB** [Tze21]. **rhencyclopropene** [DZ23]. **rheology** [NP23]. **Rhodopsins** [HREvdK<sup>+20</sup>]. **riboswitches** [AAe20]. **ribozyme** [JRS20]. **rich** [JMV21, SCCZ21]. **Riemann** [MA23a]. **right** [SCZ<sup>+21</sup>]. **Rigid** [Min20, WCD<sup>+23</sup>]. **Ring** [LJ20, AG21, Jab22b, KB22]. **rings** [DZ23, HS22, HS23]. **RISM** [CKH23, MY24, YIO20]. **RISM/3D** [MY24]. **RISM/3D-RISM** [MY24]. **RISMicCal** [MY24]. **RL** [JGK<sup>+22</sup>]. **Rn** [APR21]. **RNA** [AAe20, BVGB23, KR23, SCCZ21, TM20, WCT<sup>+23</sup>, YFH<sup>+21</sup>]. **robust** [NMF121]. **Role** [MKSS20, MAP<sup>+20</sup>, NAAP21, BVC<sup>+23</sup>, FM21, GCP22, KE23b, LKT21, MCD22, SGGG22, SNK24b, ZG21, ZOD<sup>+22</sup>]. **roles** [VV20b]. **rotamers** [PFP<sup>+21</sup>]. **rotating** [YrYqLhC23]. **rotation** [Kop22b, PGDD24]. **rotational** [PSMPB21]. **rotations** [PDL24]. **rotors** [YrYqLhC23]. **route** [SSM21]. **Roux** [IBL20]. **rovibrational** [ERVN24, IAF<sup>+24</sup>, SR23]. **RS** [MGB<sup>+22</sup>, SHHH22, VAL20]. **RS-REMD** [MGB<sup>+22</sup>]. **RSX** [RMBSPJSG24]. **RSX-QIDH** [RMBSPJSG24]. **Ru** [HSG21, ĆPP<sup>+22</sup>]. **rubber** [MML<sup>+23</sup>]. **RuBisCO** [DGSB<sup>+20</sup>, JMK<sup>+20</sup>]. **RuC** [Tze21]. **rule** [TLD<sup>+22</sup>, TTT<sup>+21</sup>]. **rung** [RMJ21]. **rung-3.5** [RMJ21]. **ruthenium** [KK23, YYS20]. **rutile** [VTdlM20].

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

[Sts20]. **saddle** [MH22]. **safe** [JRS20]. **salts** [JMV21]. **same** [Sán20]. **same-spin** [Sán20]. **Sampling** [FMFG20, RD23, AKR21, BPT<sup>+</sup>23, 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** [dMBdAVdS24, 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, dMBdAVdS24, EIT<sup>+</sup>21, KLZ<sup>+</sup>23, PDC23, PPP21, PPRS22, YC23]. **save** [POvG21]. **scalar** [RNP20]. **scale** [ARR22a, BTC24, 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, YMM<sup>+</sup>24]. **scaled** [Sán20]. **scaling** [ASW20, CC22, MKK<sup>+</sup>22, MGB<sup>+</sup>22, MZMK<sup>+</sup>21, RR22, SEZ20, ZWY<sup>+</sup>22]. **scandium** [GSSG24]. **scattering** [CV22, DHD21, MH20]. **scavenger** [Mon24]. **SCF** [HNCL24]. **SCH** [SVTK<sup>+</sup>22]. **scheduling** [MLC<sup>+</sup>23]. **Scheme** [BSL20, GRN20, BA24, FCPG20, Gao20, LLZ<sup>+</sup>23, MT20b, RH21, STR20, VWJ23, ZZ23a]. **schemes** [DO20, HD21, MPP23, SFS24, ZQ24]. **schiff** [ZRSST20]. **Schrödinger** [Nan24]. **Schwarz** [IW23]. **Science** [PAF<sup>+</sup>20, PSGL21]. **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** [ZYZ24, AFR<sup>+</sup>24a, AR20, CJHW21, KDP<sup>+</sup>22, LCP21, MLG<sup>+</sup>21b, MPR22, NBE<sup>+</sup>23, Ore24, UAC<sup>+</sup>23, WRVP22]. **Se** [JS21, KPTT21, AQMM<sup>+</sup>23]. **Search** [BW22b, BAO<sup>+</sup>20, RD24, 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]. **seen** [CCZ23]. **selected** [CN21, KZOV23]. **selected-CI** [CN21]. **selection** [BPL<sup>+</sup>22, LCP24, SKL23]. **selective** [HRTSS<sup>+</sup>20, KI24, YLZ<sup>+</sup>22, ZOD<sup>+</sup>22]. **selectivity** [BAM<sup>+</sup>24, 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** [IW24, ASW20, BUNO22b, CV22, CQSG20, CTPJH22, MAP<sup>+</sup>20, PRH20, SKKK20]. **self-assembly** [MAP<sup>+</sup>20, PRH20]. **Self-consistent** [IW24, 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, MM24]. **sensitizers** [LCP21]. **sensor** [ZRSST20]. **sensors** [MK22b]. **Separated** [BBK20, RMBSPJSG24]. **Separation** [NS22, WG20, YYZ<sup>+</sup>21, ZHG<sup>+</sup>24]. **SEQCROW** [SIW21]. **sequence** [CR24, KZOV23, KSRKS21, SBFSJMLU23]. **sequence-based** [KSRKS21]. **sequential** [GGK20]. **series** [BHR<sup>+</sup>21, PWX<sup>+</sup>20, WZW<sup>+</sup>24, ZWL<sup>+</sup>24a]. **server**

[LGD<sup>+</sup>20, MPuS<sup>+</sup>20, FPMD23]. **servicing** [TSH<sup>+</sup>23]. **Set** [XZ20, YXGZ20, BK22, Fed24, HGR<sup>+</sup>24, KS21, MM24, MCP23, SCKH21, TAC<sup>+</sup>23]. **sets** [GZFSM21, GH22b, GH23, KM24, LB21, LB22, NSH23, RNP20, SLB23, SM22a]. **setup** [CLTMd<sup>+</sup>23]. **seven** [KZJ22, ZYZ24]. **seven-electron** [ZYZ24]. **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, XIV<sup>+</sup>24]. **shell** [AME<sup>+</sup>21, GSSG24, IW24, Klo22, MB21, Sán20, SM23, PSMPB21]. **shielding** [CMG<sup>+</sup>24]. **shift** [FBP<sup>+</sup>22, TTDT20, UB20]. **shifts** [Ben22, KWX23, MPV22, ZHHS21]. **shock** [BAO<sup>+</sup>20, FVSS20]. **short** [HTFY21, SKKG22]. **short-range** [HTFY21]. **Si** [GPM21b, WMJ<sup>+</sup>22, KPR23, WTST24a, VCRP23]. **side** [BSR22, ODL20, SSS<sup>+</sup>20b]. **side-chain** [SSS<sup>+</sup>20b]. **signal** [XIV<sup>+</sup>24]. **signaling** [CDCT21]. **sil** [KDMM24]. **sil/germa** [KDMM24]. **silaboryne** [DDSM23]. **silane** [MML<sup>+</sup>23]. **silica** [MML<sup>+</sup>23]. **silica/rubber** [MML<sup>+</sup>23]. **silico** [dMBdAVdS24, LHB<sup>+</sup>24, MAI22, SEBE21, SC23, PFPD21]. **Silicon** [HZG<sup>+</sup>20, GPEK<sup>+</sup>20, PGP<sup>+</sup>21, WZW<sup>+</sup>24, ZXD20b, ZXD20a]. **silicon-based** [WZW<sup>+</sup>24]. **siloxo** [LLS<sup>+</sup>22b]. **silver** [FNPD22, Mon24, XDZ23]. **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, ZHG<sup>+</sup>24, 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, BTL24, CCZ23, DO20, EK20a, FCB23, FLT23, GGK20, HUUO23, IAS<sup>+</sup>24, JKS23, LL21a, LKM20, LSC<sup>+</sup>23, LGC21, MP24, MPOC21, MSA22a, Ngo21, NN20, NP23, PDC23, PBM21, PDL<sup>+</sup>21, POvG21, PL22, PCI23, QLC<sup>+</sup>20, RDK<sup>+</sup>22, RGGD21, SC23, SSDL<sup>+</sup>23, SKKK20, TTK23, TPB22, Tik23, WCT<sup>+</sup>23, WW24, WGKG20, WFBB22, WKD<sup>+</sup>21, Yos24, YMM<sup>+</sup>24, ZKJ<sup>+</sup>23]. **Simultaneous** [GKO<sup>+</sup>22, BMT23, WFLZ23]. **single** [AK20, BW22a, CBF<sup>+</sup>20, DLH<sup>+</sup>23, EVKL21, FMK24, 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** [VDK<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** [ENR<sup>+</sup>24, HGF20, LKM20, MAKZ23, TXJT23, VHS<sup>+</sup>24, YIO20]. **sites-based** [VHS<sup>+</sup>24]. **Si**  $\equiv$  [DDSM23]. **situ** [MC24, WKG<sup>+</sup>23]. **situation** [FNPD22]. **situations** [THLC<sup>+</sup>23]. **six** [PTP23]. **six-electron** [PTP23]. **sixth** [LB21]. **size**

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

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



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

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

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

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

**Transition** [PWW20, AR20, BW22b, CH23, DRBT24, EK20a, EK20b, HNCL24, KL20, KMR<sup>+24</sup>, MLM<sup>+24</sup>, MYYS24, NBE<sup>+23</sup>, PDC23, PTP23, PDGD23, PGDD24, PSM<sup>+20</sup>, RSHG23, SKY24, SDH23, SBB<sup>+22</sup>, SHH<sup>+24</sup>, VV20b, WW24, XZC<sup>+24</sup>, dCVARN20]. **Transition-Metal** [PWW20]. **transition-potential** [EK20a]. **transitions** [EK20c, HSG21]. **Transmembrane** [MKSS20, SSS<sup>+20b</sup>]. **transmission** [XIV<sup>+24</sup>]. **Transport** [HHL<sup>+20</sup>, YC20, LEP<sup>+21</sup>, WSV20, XZW<sup>+21</sup>, ZGZ<sup>+20</sup>]. **trapping** [ZS22]. **traversal** [BTC24]. **treat** [SSDL<sup>+23</sup>]. **treatment** [Cer22, HMK23, MM24, SLMA21]. **Tree** [AZKM22, AYO20, CN21, TIK21]. **treecode** [WKL22]. **Tren** [Ari24]. **trends** [SDK20]. **tri** [dSCCN21]. **tri-** [dSCCN21]. **Triacylglyceride** [CST23]. **trialkyl** [SGRN24]. **triangulation** [WK21]. **triazole** [KGD<sup>+21</sup>]. **triazolotetrazine** [KZP22]. **Trichoderma** [HYA<sup>+20</sup>]. **tricoordinated** [THLC<sup>+23</sup>]. **triclesyl** [HUUO23]. **trifluoro** [SMB<sup>+23</sup>]. **trifluoropropene** [BR23]. **trimeric** [PDC23]. **trimethylphosphine** [CS20]. **trioxides** [KZP22]. **tripeptide** [OAC23]. **tripeptides** [OAC23]. **triphosphate** [XZX<sup>+22</sup>]. **TriPip222** [Ari24]. **triple** [DTA21, LB21, LB22, SLB23, ZMH<sup>+21</sup>]. **triple-zeta** [LB21, LB22, SLB23]. **Triplet** [HFPS20, BGPR24, ERVN24, MdSJ<sup>+23</sup>]. **tris** [AS20, MCD22]. **tropolone** [OSHT20]. **truncated** [GJMPVR<sup>+20</sup>]. **Truncation** [GJMPB<sup>+20</sup>, NAN<sup>+23</sup>]. **tryptophane** [CGMRVBAI22]. **tuberculosis** [RKC21, RDK<sup>+22</sup>]. **tumors** [CM20b]. **Tuning** [BKM21, BBK20, Cer22, CCPR24, MP23, ARR22a]. **tunneling** [Nan24, OSHT20, SRB21]. **TUPÁ** [PL22]. **tutorial** [PSW<sup>+24</sup>]. **Two** [LHC<sup>+21</sup>, SNK24b, YrYqLhC23, BPDG21, FCB23, HYA<sup>+20</sup>, IN23a, IWN24, KGS<sup>+21</sup>, KL20, PTP23, dSSCC24, STB<sup>+20</sup>, VWJ23, Wan23, YAO20]. **Two-** [SNK24b]. **two-body** [VWJ23]. **two-component** [IWN24, KL20]. **two-dimensional** [dSSCC24, STB<sup>+20</sup>]. **two-electron** [IN23a, PTP23]. **Two-layer** [YrYqLhC23]. **type** [ABZ20b, BVC<sup>+23</sup>, FV20, LL21a, LLKS23, MFS22, WKCP21, KUNT20]. **Type-1** [KUNT20].

**U** [SGRN24, SB20]. **ubiquitous** [PRF20]. **UCI** [BEKM24]. **UG** [SCCZ21]. **UG-rich** [SCCZ21]. **UiO** [FP23]. **UiO-66** [FP23]. **Ullmann** [LHG<sup>+23</sup>]. **ultra** [MLX<sup>+24</sup>, SKKG22]. **ultra-fast** [MLX<sup>+24</sup>]. **ultra-short** [SKKG22]. **ultrafast** [BBL<sup>+22</sup>, CCPR24, LAM<sup>+23</sup>]. **ultrashort** [Jab22b]. **umbrella** [Ngo21, SSS<sup>+20a</sup>]. **Uncertainty** [HM21, CR24]. **unconstrained** [CRT<sup>+21</sup>]. **Uncovering** [GM22, TLD<sup>+22</sup>]. **underlying** [ONA<sup>+20</sup>, WFBB22]. **Understanding** [KZJ21, MGCM21, NVBG23, SMB<sup>+23</sup>, CX23]. **unique** [DYGM21, KLZ<sup>+23</sup>]. **Unitary** [SBG20]. **Units** [AD20, GCL<sup>+20</sup>, Ari24, DWZ22]. **universal** [LGM20, LGM22]. **Unlocking** [GUCCR20]. **Unprecedented** [JFZ<sup>+20</sup>]. **Unraveling** [BRNB21, FMK24, JWS<sup>+24</sup>, KS24]. **UNRES** [SSDL<sup>+23</sup>]. **unsaturated** [BA24, MLGY24]. **unusual** [LML<sup>+23</sup>]. **Unveiling** [IMT<sup>+21</sup>]. **UO** [BEKM24]. **updated** [MT20b]. **upon** [EK20c, YOCMA23]. **Uranium**

[BEKM24]. **Uranium-based** [BEKM24]. **uranyl** [PB20]. **usage** [KF24]. **Use** [Fed24, BBB<sup>+</sup>23, CK22, COK22, POvG21]. **useful** [ZGZC20]. **user** [SKS21, ZK23]. **user-friendly** [SKS21, ZK23]. **Using** [CTPJH22, GCL<sup>+</sup>20, KUNT20, LJ20, MK22a, VAL20, WZZ<sup>+</sup>20, AV20, Ano24a, BS23, BHR<sup>+</sup>21, JGdC<sup>+</sup>23, BSL20, BSF20, BF22, CV22, CGSP24a, CQSG20, CST23, DHD21, DGSB<sup>+</sup>20, GNK<sup>+</sup>23, GK24, HUUO23, HPM<sup>+</sup>21, IN23a, JGGPN21, KWX23, KMR<sup>+</sup>24, KLP<sup>+</sup>22, KSRB<sup>+</sup>21, KB22, KdILC22, LA20, LRF<sup>+</sup>21, LGC21, LWLC21, LDT<sup>+</sup>22, MPP23, MN20, MIP<sup>+</sup>22, MEKH22, MA23a, MC24, MSS20, NS22, OC23, PJJL23, PAS<sup>+</sup>20, PWX<sup>+</sup>20, PDP<sup>+</sup>24, PFPD21, QLW<sup>+</sup>22b, RR22, SW21, SK23, SEZ20, SSB<sup>+</sup>20, SCCZ21, SHH<sup>+</sup>23b, TIK21, TLD<sup>+</sup>22, Tou21, WKCP21, WMZJ20, WCY<sup>+</sup>24, WdGG24, WKG<sup>+</sup>23, Yos24]. **USPEX** [VWFR21]. **utilized** [GM22]. **utilizing** [HD21]. **UV** [CWZD20, LWLC21, TMO<sup>+</sup>21]. **UV-Vis** [CWZD20, LWLC21, TMO<sup>+</sup>21].

**V** [MNH21]. **v2.0** [GJMPVR<sup>+</sup>20]. **Valence** [BJ22, CB20, LB21, LB22, NHFS21, PDGD23, SVTK<sup>+</sup>22, SLB23, XCJ20]. **Validation** [BLP20, DPSG20, WZZ<sup>+</sup>20, LCC<sup>+</sup>21]. **validations** [GP21, KGD<sup>+</sup>21]. **validity** [PRF20]. **value** [MT20b]. **values** [SHHH22]. **Vanadium** [SB20]. **van't** [ZXD20b, ZXD20a]. **variability** [YBS<sup>+</sup>20]. **variable** [BPT<sup>+</sup>23]. **variant** [AB AQ<sup>+</sup>23]. **variants** [KLZ<sup>+</sup>23]. **Variation** [JS21, HKFT21]. **Variational** [dCVARN20, GH22b, GH23]. **Variations** [FMFG20]. **varying** [DB23]. **VASP** [VWFR21]. **VEGF** [KR23]. **verification** [HNCL24]. **versatile** [FPMD23]. **version** [CSG<sup>+</sup>21, DKB23]. **Versus** [LR20, BBBP<sup>+</sup>23, CMO<sup>+</sup>24, MJS<sup>+</sup>23, MP23, NYM22, SK23, SM23]. **Vertical** [NRH<sup>+</sup>20, FCB23]. **VI** [SGRN24]. **via** [ARR22a, ABAQ<sup>+</sup>23, CB20, IW23, IMT<sup>+</sup>21, KZJ22, KI24, LSC24, Ngo21, PWW20, PCB<sup>+</sup>24, RKC21, SZL23, TM20]. **vibration** [Kop22b]. **vibration-rotation** [Kop22b]. **vibrational** [BEKM24, CV22, FDK22, FAK24, JMV21, MR21, MPR22, PCI23, Shi22]. **Vibrationally** [CS23, AS21]. **Vibrationally-resolved** [CS23]. **vibronic** [Tou21]. **view** [PGP<sup>+</sup>23]. **viewpoint** [NHFS21]. **viewpoints** [MGCM21]. **VIM** [KGD<sup>+</sup>21]. **VIM-2** [KGD<sup>+</sup>21]. **Vina** [PNT<sup>+</sup>22]. **viologen** [OAN<sup>+</sup>23]. **viral** [GG22]. **virtual** [LKM20, MLG<sup>+</sup>21b, MSL<sup>+</sup>20]. **Virus** [KUNT20, LSC<sup>+</sup>23, MPuS<sup>+</sup>20]. **virus-like** [LSC<sup>+</sup>23]. **vis** [TMO<sup>+</sup>21, CWZD20, LWLC21]. **visual** [LC22]. **Visualization** [AKR21]. **voltage** [XAD20]. **voltage-dependent** [XAD20]. **Volume** [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, GCL<sup>+</sup>20, RPD<sup>+</sup>20b]. **volumes** [BBSFA22]. **Voronoi** [NVBG23]. **vs** [Ano24a].

**W1X** [CK22]. **Waals** [BS23, EK20b, POPGS22, YW20]. **wales** [CTBB20].

walled [BW22a, CBF<sup>+</sup>20]. **Water** [CCZ23, HRT<sup>+</sup>20, MM20, Bal20b, BCN22, CVGVN<sup>+</sup>20, ĆPP<sup>+</sup>22, DTA21, DHN<sup>+</sup>21, GSH23, GP21, KEK23, LLZ<sup>+</sup>23, MPOC21, MKB<sup>+</sup>21, PLP<sup>+</sup>20, PGH24, PM21, RPD<sup>+</sup>20a, SHH<sup>+</sup>23b, VCRP23, VV21, YYS20, LSC24]. **Water/organic** [CCZ23]. **waters** [ZOD<sup>+</sup>22]. **wave** [CV22, NEG<sup>+</sup>20, SWM<sup>+</sup>20b, WMZJ20]. **wavefunction** [SM20]. **wavefunctions** [ALA20]. **Waves** [WG21, FVSS20, MN20, Wan21a, Wan21b]. **weakly** [Brz23]. **web** [LGD<sup>+</sup>20, MPuS<sup>+</sup>20]. **weighted** [GJMPVR<sup>+</sup>20, MCP23, MA23a, MT20b, RD23]. **weighted-core** [MCP23]. **well** [KN21]. **well-sliced** [KN21]. **whether** [APS20]. **Which** [Wan21a, Wan21b, WG21]. **wide** [BdLC21]. **wild** [CSP20]. **wires** [AMF<sup>+</sup>20, LAM<sup>+</sup>23]. **Withania** [PPP21]. **Within** [SBG20, BPT<sup>+</sup>23, CVGVN<sup>+</sup>20, Cer22, GRN20, IYI<sup>+</sup>20, IW24, JC20, OAC23, PW20, SMB<sup>+</sup>23]. **without** [VZG<sup>+</sup>24, WFBB22, WKG<sup>+</sup>23]. **word** [QLW<sup>+</sup>22b]. **work** [CPG21, ZGZC20]. **workflow** [MKB<sup>+</sup>21, SYS<sup>+</sup>21]. **would** [APS20]. **Wouthuysen** [IWN24]. **writing** [VAP<sup>+</sup>21].

**X** [APR21, SCC<sup>+</sup>22, LDT<sup>+</sup>22, AQRA<sup>+</sup>23, AQMM<sup>+</sup>23, ABAQ<sup>+</sup>23, EK20a, FB20, Kop22a, SHP<sup>+</sup>23, TTT<sup>+</sup>21]. **x-phenylenediamine** [LDT<sup>+</sup>22]. **X-ray** [EK20a, FB20]. **XCl** [AQMM<sup>+</sup>23]. **Xe** [RNP20]. **XEDA** [TSZ<sup>+</sup>21]. **xenon** [GH22b]. **XGBoost** [DPY<sup>+</sup>22]. **XGBoost-based** [DPY<sup>+</sup>22]. **XMoO** [AQRA<sup>+</sup>23]. **XP** [CC22]. **XP-PCM** [CC22]. **xB** [MKB<sup>+</sup>21, OM22].

**YF** [AWK<sup>+</sup>23]. **yield** [DPY<sup>+</sup>22]. **yields** [SKGG23, TCS<sup>+</sup>21a, YGG<sup>+</sup>23]. **yl** [MIP<sup>+</sup>22]. **ylide** [SMB<sup>+</sup>23]. **yttrium** [GSSG24].

**zeolite** [NS22]. **zeta** [LB21, LB22, SLB23]. **Ziff** [VFCG20]. **zigzag** [SPT21]. **Zinc** [MK22b, YrYqLhC23]. **Zintl** [LXP<sup>+</sup>22]. **zirconocene** [MLB<sup>+</sup>23]. **Zn** [AQRA<sup>+</sup>23, BD22, GP21, MAKZ23]. **ZnO** [GAG20]. **Zr** [DBE20]. **ZrS** [DLH<sup>+</sup>23]. **zwitterionic** [LEP<sup>+</sup>21, MPOC21]. **ZZS** [WRVP22].

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- [Ano21g] **Anonymous:2021:IIh**  
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- [Ano21h] **Anonymous:2021:IIi**  
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- [Ano22h] **Anonymous:2022:IIh**  
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- [Ano22k] **Anonymous:2022:IIk**  
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- [Ano22m] **Anonymous:2022:IIm**  
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- [Ano22n] **Anonymous:2022:IIn**  
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- [Ano22o] **Anonymous:2022:IIo**  
Anonymous. Issue information. *Journal of Computational Chemistry*, 43(15):995–999, June 5, 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 JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- Anonymous:2022:IIq**
- [Ano22q] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(17):1135–1139, June 30, 2022. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- Anonymous:2022:IIr**
- [Ano22r] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(18):1201–1205, July 5, 2022. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano22s] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(19):1271–1275, July 15, 2022. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- Anonymous:2022:IIt**
- [Ano22t] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(20):1329–1333, July 30, 2022. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano22u] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(21):1389–1393, August 5, 2022. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- Anonymous:2022:IIv**
- [Ano22v] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(22):1459–1463, August 15, 2022. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano22w] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(23):1525–1529, September 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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- [Ano22-29] **Anonymous:2022:IIbc**  
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- [Ano22-30] **Anonymous:2022:IIbd**  
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- [Ano23c] **Anonymous:2023:IIc**  
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- [Ano23e] **Anonymous:2023:IIe**  
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- [Ano23j] **Anonymous:2023:IIj**  
Anonymous. Issue information. *Journal of Computational Chemistry*, 44(10):1011–1015, April 15, 2023. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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- [Ano23-28] **Anonymous:2023:IIbb**  
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- [Ano23-29] **Anonymous:2023:IIbc**  
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**Anonymous:2023:IIbf**

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- [Ano24b] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(1):1–5, January 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

**Anonymous:2024:IIb**

- [Ano24c] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(2):65–69, January 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

**Anonymous:2024:IIc**

- [Ano24d] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(3):135–139, January 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

**Anonymous:2024:IIId**

- [Ano24e] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(4):193–196, February 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

**Anonymous:2024:IIe**

- [Ano24f] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(5):233–237, February 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

**Anonymous:2024:IIIf**

- [Ano24g] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(6):301–305, March 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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- Anonymous:2024:IIl**
- [Ano24m] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(12):821–826, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- Anonymous:2024:IIm**
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- Anonymous:2024:II n**
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- [Ano24r] **Anonymous:2024:IIq**  
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