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(n, m) [RA20]. $(n = 8, 10)$ [MI20]. $(x + y + z = 6)$ [KYL+20]. 1 [MSADA21]. 12 [AJC+21, ZZZ20b]. 15 [JZL+21]. 18 [DYG21, GYC20]. $1s2s3s$ [NdVVT22]. $1s^2$ [NZAH21]. 2 [BRB+21, EM21, KMK21, MKKA21, WWZ+20, WAW+21]. 3 [JXL+21, MSS22, SRS21]. 38 [GZWL22]. $3d$ [DRV20]. $3z$ [SK21]. 4 [MSADA21, YST+21]. $4d$ [DRV20]. $4f$ [sLhZX+22]. $4f \rightarrow 5d$ [GYC20]. 5 [BSH+21, JXL+21, LSS+21]. $5f$ [sLsHtW+23, sLLqX+23]. 6 [BA21, MSS22, QOM+20, ÜB20]. 60 [GZWL22]. $6\pi/2\sigma$ [ZFB+20]. 7 [MSS22]. 8 [MSS22]. $[3 + 2]$ [MSADA21, TXW+20]. $[4 + 1]$ [KZ21, YYL21]. $[4 + 2]$ [LZ21, YYL21]. $^{+}$ [Ari21, ABDD22, BA21, FK20, Iri21, JWZZ20, KWWZ20, KC23, MSS22, MKD21, MM20, PCKP20, Shi21, SPR22, Wan21]. $^{+}_{2}$ [GRLH21]. $^{-}$ [BFW+22, HDF+21, THL+21, WWWC21]. ^{1} [Cha21a, SSK20, SPR21, SPR22]. ^{13} [Cha21a, GMRKMCMC21, SSK20, SK21]. ^{19} [GZC21]. $^{2+}$

[CLC+21, FAJOF20, VCM+21, WDS+20]. $^{2+/3+}$ [RR21]. $^{2-}$ [SGWW22]. $^{2}\Pi$ [ASO+22]. ^{3} [BESG22]. $^{3}+$ [SMK+23, MAHRA+21, SMK+23, TSHRS+20]. ^{31} [GZC21]. $^{4+}$ [WWKH22]. ^{III} [SKR+21, WSSD21]. ^{IV} [SKR+21]. $^{n+}$ [QOM+20]. $^{q+}$ [MSS22]. ^{t} [VOK+20]. $_{0}$ [WAM+20]. $_{0.5}$ [KC23, YFX+22]. $_{1}$ [NYX+21, WAM+20, XPZ20]. $_{1-8}$ [Kov20]. $_{1-x}$ [ARRB+21, BB20, MTA+22, TMH21, ZYZ+21b]. $_{11}^{-1}$ [Yan20]. $_{12}$ [GZWL22, KMG22, PL20, SYD+23, YFX+22, dPZFM+22]. $_{12-k}$ [SBKT23]. $_{17}$ [SYD+23]. $_{18}$ [ILPY+23, JXYL20]. $_{2}$ [AAJ+23, AII21, AMK+20, ARRB+21, BFW+22, BBAA21, BZP+20, BB20, CSL+23, CXZ+21, CZGW22, CWL+22, CLLC21, DRV20, EGLJQ+21, EB22, FK20, FAB+23, FGW+22, GNC20, GSRG22, GGUU21, GUUG23, HNO+21, HLL20b, HYC+21, HZC21, IMJ21a, JZL+21, KDY+22, KWWZ20, Kan21, Kan22, KHK+23, Kov20, KC23, LLLL20, LLZC20, LHZG23, LYW+20, LHL+21, LWH+21, LDS+23, LCY+23, LZL+21, LXWZ21, LZZ+20, MSS20, MIA23, MZ23, MKM+20, MKD21, MZ21, MHS21, MBM+21, MHG+23, MAK+22, NLA+21, dRNS21, NHH22, dAOdASP+20, ONH+21, OGSPP+22, PAS+21, Pan20, PASS21, PVR20, PZGH+20, PLZT22, PRC23, PP21, QDC+22, QdOdMC+21, RCM+22, RS21, RS23, RKA+21, RINHY20, RHS+21, RSM+22, RNRBFC21, Roy20, SSIE20, SSEI21, SSIE21, SIM23, SPF+22, SGWW22, SUG20, SCY+23, TXW+20, TWT+21, TCX+22, UP20, ÜB20, VNK+23, WLP+20, WDS+20, WXL+21, WZL+21, WXHX22, WCM+23]. $_{2}$ [WCZ+20, WOE+22, WAW+21, XPZ20, XHX+20, XQJ+21, XWS+22, Yan21, Yan20, YST+21, YZD+21, YCL+23, YZL+21b, ZZZ+20a, ZCL+22, ZZLY22, tZNb+22]. $_{20}$ [Ari21, JXYL20, TWT+21]. $_{20-k}$ [SBKT23]. $_{21}$ [ELH20]. $_{2}^{(-1)}$ [GNC20]. $_{2}^{+}$ [Dau21, MM21]. $_{2}^{2+}$ [Yan20]. $_{2d}$ [GMRKMCMC21]. $_{2n}$ [LCT+22]. $_{3}$ [AAM+20, BPB+20, CSL+23, EGLJQ+21, FGW+22, JXYL20, JZL+21, KDY+22, LFRTRP+20, LDS+23, LFMF23, LZZ+20, MJA20, MSS20, MAHRA+21, MZ23, MHS21, MT21, MTA+22, MT23, NG20, ORL+20b, PAS+21, Pan22, PPCF+20, PCKP20, PLT+20, QOM+20, RINHY20, RMeH+20, RR21, SUG20, SBG21, SMK+23, SXTZ23, TWT+21, TCX+22, WDS+20, WXL+21, WZL+21, XFW+20, fXmTlS+23, YCPW20, YZL+21b, YHZ+22, ZZZ+20a, ZFB+20, ZHG+22, ZQZ+23b, ZHS21]. $_{36}$ [GMRKMCMC21, Tia21]. $_{3}^{+}$ [HDF+21, ZFB+20]. $_{3h}$ [PCKP20]. $_{4}$ [AAJ+23, CZC+23, EB22, KHH+21, KHK+23, KMG22, KS21, MSS20, MHG+23, PPCF+20, PC22, RINHY20, RR21, SGWW22, THL+21, VNK+23, WDS+20, WWZ+21, YZL+21b, YCSK20, ZWZB23]. $_{4-n}$ [OGSPP+22]. $_{49}$ [JXYL20]. $_{4}^{+}$ [WAW+21]. $_{4}^{-}$ [WDS+20]. $_{4}^{2-}$ [HOVG20b]. $_{5}$ [ASO+22, CYL+23, Kan21, LYPD23, PP21, SRS21, WWWC21, YCPW20]. $_{5.5}$ [PZGH+20]. $_{58}$ [JXYL20]. $_{6}$ [AMK+20, ASO+22, FAB+23, GSRG22, ILPY+23, LYPD23, RKA+21, RSM+22, WJF+21, YCSK20, ZCL+22]. $_{6,7}$ [RG20]. $_{60}$ [ABDD22, CCZ20, DFK20, GMO+20, MZ21, SBAT23]. $_{60}^{-}$ [HL20]. $_{6h}$ [GMRKMCMC21]. $_{7}$ [CYL+23]. $_{70}$ [GMO+20]. $_{8}$ [CYL+23, LWC+21, MZD+20, QOM+20, SRS21]. $_{9}$ [ZWZB23]. $_{92-x}$

[MZD+20]. $_a$ [PS23a]. $_k$ [SBKT23]. $_m$ [PP21, SNL+23]. $_n$ [AJC+21, FPdS21, GNC20, GZWL22, JZL+21, MOB21, OGSPP+22, SNL+23, SP20b, TSS+23, Yan21, ZZZ20b]. $_{n=1--4}$ [FK20]. $_{n=1-4}$ [FK20]. ^+_n [ÜB20]. ^-_n [WYL22]. $^{-/0/+}_n$ [TT21b]. $^{0/-}_n$ [DCY21]. $^{0/-}_n$ [DYG21, GYC20]. $_X$ [APR20, Kid21, ARRB+21, BB20, GTC+23, KYL+20, MZD+20, MTA+22, QOM+20, TMH21, WLP+20, YST+21, ZYZ+21b]. $_y$ [GTC+23, KYL+20]. $_z$ [KYL+20]. α [JAZ+20, YZL+21b, ZXS20]. β [BSH+21, KLT21, RKG21, ZLH20a]. $\mathcal{L}_q$ [SSD22, SD23]. $\cdot$ [SKR+21, WLLS21, WLLS21]. $\cdots$ [MOB21, SLL+22]. Δ [JXM22]. η' [LYPD23]. g [JAZ+20]. γ [SUG20, Sur20, Sur22]. J [OR21]. k [SBKT23, Zhu21, ZZL20b]. l [MWCJ23, PGROM20]. $\lambda = 0, \pm 1$ [LDK23]. λ^3 [NHNO20]. $m \neq 0$ [CSS+21]. N [DDSB22, KKK23, LLZ+20, PM20, SF20a, TXW+20, DCY21, LCT+22, LDK23, MI20, MOB21, PSJ22, SMS23, TSS+23, TT21b, WYL22]. $N + 1$ [KKK23]. $n = 0, 1, 2, 3, 4$ [OGSPP+22]. $n = 1$ [JZL+21, ZZZ20b]. $n = 10$ [DYG21]. $n = 2$ [AJC+21, ÜB20]. $n = 30$ [GZWL22]. $n = 5$ [PSJ22]. $n = 6$ [GYC20]. $n{:}\, m \geq 2{:}\, 1$ [SNL+23]. $n \to \pi*$ [CP23]. ω [DPC+20]. π [HLL20b, HFF22, LYT+20, LL21, MPBL23, OR21, PGPHAPM20, SSIE21, SLL+22, VM20, ZIA20, ZL21]. q [Lom21, PGROM20, SD23]. $q = 1$ [MSS22]. $q = 2$ [MSS22]. s [KKK23]. σ [BSMB23, KSP20, LL21, VM20]. $\Sigma 3[110](111)$ [PP23]. t [CMM+22]. $\rightarrow$ [JWZZ20, WY20, WCZ+20]. x [APR20, BB20]. $X^2\Pi$ [KRS+21].

&K [TWT+21].

-1 [LMAA23]. **-1H-azoles** [QLGZ23]. **-5** [BRB+21]. **-A-D** [XPZ20]. **-acceptor** [LYT+20]. **-acylhydrazones** [TXW+20]. **-Al** [YZL+21b]. **-alanine** [JAZ+20]. **-aromatic** [JS21]. **-based** [XZ20, Üng23, dRNS21]. **-bound** [PGROM20]. **-bromanes** [NHNO20]. **-bromochloroethane** [WAW+21]. **-butadiene** [SRS21]. **-butene** [WWZ+20]. **-butyl** [CMM+22]. **-BX** [PVR20]. **-carbamido-1** [EM21]. **-catalyzed** [WLH+20, TXW+20]. **-centered** [SF20a]. **-conjugated** [HFF22, OR21, SSIE21, ZIA20]. **-coupling** [OR21]. **-Cu** [LYPD23]. **-cyclization** [YCSK20]. **-cyclodextrin** [BSH+21]. **-deformed** [PGROM20]. **-diborene** [SLL+22]. **-diketones** [RKG21]. **-directed** [WSSD21]. **-edge** [RG20]. **-electronic** [Kha23]. **-enylidene-malonitrile** [BRB+21]. **-exponentials** [Lom21]. **-Fe** [SUG20]. **-fluorouracil** [BSH+21]. **-graphene** [MIA23]. **-graphs** [RA20]. **-heterocyclic** [DDSB22, LLZ+20, PM20]. **-hole** [HLL20b, KSP20, LL21, VM20, ZL21]. **-hydroxylmethylfurfural** [LSS+21]. **-isoxazolines** [MSADA21]. **-lactamase** [KLT21]. **-lactide** [MWCJ23]. **-mediated** [PD22]. **-methyl** [MSM+20]. **-Mo** [PP21]. **-NH** [PLT+20]. **-nitro-1** [JXL+21]. **-norms** [SD23]. **-one** [JXL+21]. **-oxide** [MSADA21]. **-phenyl** [LMAA23]. **-photon** [Dau23]. **-poly** [LMAA23]. **-profile** [BSMB23].

-propylamine [SMS23]. **-pyrroline-** [MSADA21]. **-rich** [MZ21]. **-S** [SK21]. **-SCF** [JXM22]. **-sequestration** [QdOdMC+21]. **-tensors** [JAZ+20]. **-TPA** [HFF22]. **-tricyclic** [SWXM23]. **-type** [KKK23, Pan22]. **-uniform** [Zhu21, ZZL20b]. **-valence** [QOM+20]. **-vinylsilane** [ZXS20].

/2 [KKK23]. **/2-site** [KKK23]. **/CNT** [SUG20]. **/D** [GMRKMCMC21]. **/DMSO** [VOK+20]. **/doped** [EGLJQ+21]. **/doped-carbon** [EGLJQ+21]. **/Eu** [LNC+23]. **/F12c** [WWF23]. **/Fe** [MGK23]. **/graphene** [MI20]. **/M** [LZZ+20]. **/NiI** [MKM+20]. **/organic** [NLA+21]. **/S** [WAM+20]. **/SiO** [WLP+20].

1-54 [RPT21a]. **1.0** [Boz21]. **11/12** [SLL+22]. **12-hexaazaisowurtzitane** [ZGCF20]. **12-hexanitro-2** [ZGCF20]. **120** [Sur22]. **121** [Ano22a]. **1234ze** [HYHW22]. **15-19** [Yan21]. **19** [KAA21, LAAP21, RNH23]. **1D** [CSK21, WZ21]. **1H** [KPTL23, QLGZ23]. **1H-imidazol-2-yl** [KPTL23].

2 [KMK21, PPR21, ZQZ+23a, Cha21b, KPTL23, TCL+21, YCSK20]. **2-** [BRB+21, PPR21, ZWL22]. **2-3-** [BRB+21]. **2-amino-2-oxyethoxy** [ZWL22]. **2'-bipyridyl-embedded** [ZQZ+23a]. **2-dimethylcyclohexyl** [BWLZ22]. **2-ethyl-hexyloxy** [LMAA23]. **2'-hydroxyphenyl** [KMK21]. **2-methoxy-5-** [LMAA23]. **2-methoxyethyl** [YST+21]. **2-methyl-1** [SRS21]. **2-phenylindol** [BSMI23]. **2-R-C** [YCSK20]. **2-site** [KKK23]. **2C9** [CS23]. **2D** [CRC21, ISL+23, LK21, RMLPGHP20, SDL+23, WZ21]. **2D/1D** [WZ21]. **2H** [LZ21]. **2H-azirines** [LZ21]. **2x** [JLWH23].

3 [LZS20, EM21]. **3'-** [LZS20]. **3-cyclohexanedione** [MOB21]. **3-dimethylcyclohexane** [BZW+21]. **3-enynes** [YYL21]. **3-hexafluoro-1-propene** [LZL+23]. **3-hexylthiophene** [LMAA23]. **3-indandione** [EM21]. **3d** [GRZ+21, GN21a]. **3H** [ZZXT21]. **3H-tetrazolo** [ZZXT21].

4 [PPR21, SYT+21]. **4-acyl-1-sulfonyltriazoles** [WLH+20]. **4'-amino-2'-hydroxyphenyl** [PPR21]. **4-b** [PGPHAPM20]. **4-cyclo-addition** [JJJM21]. **4-difluoro-crotonaldehyde** [CMM21]. **4-dimethylaminophenyl** [BRB+21]. **4-dimethylcyclohexane** [BZW+21]. **4-dione** [LZS20]. **4-dioxopyrimidine** [BY23]. **4-dithiafulvene** [ZKP22]. **4-hexadienal** [SYT+21]. **4-hexafluoro-** [WWZ+20]. **4-phenylene** [LZS20]. **4-phenylene-vinylene** [LMAA23]. **4-triazine** [LNC+23]. **4-triazol-** [JXL+21]. **4d** [RHS+21].

5- [HH23]. **5-d** [ZZXT21]. **5-dimethyl-** [KMK21]. **5-dimethylcyclohex-** [BRB+21]. **5-hydroxymethylfurfural** [DYZ+23]. **5-tetrazine** [ZJW+21]. **5-tetrazines** [HH23].

6-bis [KPTL23]. **6-trinitrophenyl** [QLGZ23].

7 [SWML23, ZZLY22].

8 [RDMF21]. **8-hydroxyquinoline** [SFPH22, UHK+22].

= [AMK+20, Ari21, APR20, AMM21, BB20, CZGW22, DCY21, FAB+23, GGUU21, GUUG23, HBB+21, HDF+21, JWZZ20, KLRS22, KHK+23, Kid21, KC23, LMM+22, LCT+22, LYW+20, LDK23, MZ23, MOB21, MBM+21, MEWD20, MHG+23, NG20, dAOdASP+20, OMA21, PAS+21, PASS21, PVR20, PZGH+20, PCKP20, QOM+20, RKA+21, RMeH+20, SPF+22, SG22, SBKT23, SGWW22, Shi21, SMK+23, SYD+23, TSS+23, Tia21, TT21b, WYL22, WXHX22, XFW+20, XL22, Yan21, Yan20].

A-D-A [GXL+22]. **Ab-initio** [PSN23]. **ABC** [LYFL21]. **abilities** [THS20]. **Ability** [dPZFM+22, hHNRA23, NHH22, ZQZ+23b]. **absorbing** [BAM20, JBPV21]. **absorption** [BWBR21, GA20, HSV22, HP21, INV22b, KMK21, KK21, KLK21, MSOA23, RG20, STI20, XBL23]. **absorptive** [PAS+21]. **ABX** [BPB+20]. **AC** [WXHX22]. **Accelerating** [AR22, WV21]. **Acceleration** [GKK21]. **acceptor** [BSS21, CZW21, GXL+22, KMH+20, LFRTRP+20, LYT+20, PGPHAPM20, ZAB+23]. **acceptors** [KSM+23, SSS23]. **account** [XHS+23]. **accounting** [ZMOE23]. **accuracy** [GZC21, KRS+21, ÜB20]. **Accurate** [MRI20, WWL21, ZYZ+22, KMK21, KV23, KAG+20, KK23b, NdVVT22, OB21b, TdV21, TVdVN21, TVdVN22, VKK+21, XHS+23]. **acetate** [ZPS+20]. **acetic** [ZWL22]. **acetonitrile** [MFC20a]. **acetylene** [AKKN20, LK21, VOK+20]. **acetylenes** [MSADA21]. **achievable** [KM21a]. **Achievement** [GG22]. **Achieving** [WLY+20]. **acid** [FFBH21, LYT+20, LMAA23, MBR21a, MA23, Roy20, RED21, SDL+22, SXTZ23, SLdS20, TLT+22, WWWC21, WCZ+20, ZWL22]. **acid-base** [WWWC21]. **acid-based** [FFBH21]. **acid-methotrexate** [MA23]. **acidic** [LZL+21]. **acidity** [PVR20]. **acids** [BVT20, HYY20, LC20, MZXL21, ZLT+20]. **acridone** [NTND23]. **acrylic** [SXTZ23]. **actinide** [KKH21]. **actinides** [WTC+23]. **activated** [KWWZ20, KK23a, NHNO20]. **activation** [dSFdSdMdM20, LWR21, PPCF+20, QDJY23, STF21]. **active** [CN21, GKPK21, HP21, LMAA23, MWBQ20, WFG+21, YXKJ21]. **activities** [RHS+21]. **Activity** [RSD21, BSMI23, CSL+23, CZJ+23, GOS20, KS23, YCSK20, dPZFM+22]. **actually** [Cio22]. **acyl** [WLH+20]. **acylhydrazones** [TXW+20]. **adamantadine** [Bra21]. **adamanzane** [RMS+23]. **adapted** [AIB21, UR23]. **Adaptive** [KCM+23, DGA23]. **added** [RINHY20]. **addition** [DYK22, JJJM21, LLZ+20]. **additive** [LAAP21]. **additives** [UBV+21]. **adducts** [MGK23, ZPS+20]. **adenine** [MHD20]. **adenine-thymine**

[MHD20]. **adenosine** [SASA21]. **adhesion** [SPF+22]. **adiabatic** [CMM21, Dau23, MM21, TPB+20]. **adjusting** [LNC+23]. **ADMET** [KB23, PB23, TB22]. **adsorbed** [DK21, HLZZ23]. **adsorbents** [FAJOF20]. **Adsorption** [HYY20, ID21, THL+21, WTC+23, ARBM21, AR22, CXZ+21, CZC+23, DJC21, GTAL23, HLL+23, JXYL20, LQZ+21, QDC+22, RBJ21, RDMF21, STI20, SBJ20, WXL+21, XCZ+21, YZL+21b, ZL23]. **adsorptivity** [HLL20b]. **advanced** [MTA+22]. **Advances** [BGM+23, PAS+21, SF20b]. **aerosol** [JLWH23]. **aerosols** [LRG+20]. **affect** [KSPG23]. **affecting** [SIM23]. **affinity** [ARBM21, TD22]. **Ag** [GSRG22, LYW+20, HLZZ23, XL22]. **against** [TB22]. **AgBiBr** [ZCL+22]. **agent** [HYC+21]. **aggregates** [CRKMC21]. **aggregation** [SYL+21]. **aggregation-induced** [SYL+21]. **Aharanov** [KASAK23]. **Aharanov-Bohm** [KASAK23]. **Aharonov** [GN21b, WOE+22]. **AIMD** [ZKP22]. **air** [BSS21]. **Al** [MBM+21, SYD+23, ER22, KYL+20, LMM+22, LLW+21, MWC+21, RS21, TSHRS+20, WWM+22, YZL+21b]. **Al-doped** [ER22]. **alanine** [JAZ+20]. **AlB** [FGW+22]. **AlC** [ARRB+21]. **alchemy** [GKK21]. **alcohol** [LWW20]. **alcohols** [LLLL20]. **alcoholysis** [CLL23]. **aldehydes** [HZZZ22, LLQ+21]. **Alder** [ABDD22]. **aldimine** [LLZ+20]. **Algebraic** [SSD22]. **algorithm** [BSMI23, CN21, MSI22, YHW+23]. **algorithm-multiple** [MSI22]. **alicyclic** [LPH22]. **aliphatic** [LC20, LNC+23]. **alkali** [FK20, GTAL23, HDF+21, LLLL20, MCP+20]. **alkali-** [MCP+20]. **alkaline** [LL21, MCP+20, RMS+23]. **alkaline-earth** [LL21]. **alkaline-earth-doped** [MCP+20]. **alkaloid** [MI20]. **alkaloids** [SSK20]. **alkanes** [SC21]. **alkenes** [LG21]. **alkenylation** [WHYL21]. **alkyl** [CLW21, CMM+22, KSPG23]. **alkylamine** [QDJY23]. **alkyne** [JRA21]. **alkynes** [PPCF+20, WHYL21, ZXS20]. **all-inorganic** [ZZLC20]. **allotropes** [PNC20]. **alloy** [LSS+21, Rac21, RSD21, ZYZ+21b]. **alloying** [DPC+20, PL20]. **alloys** [BB20, GGUU21, GUUG23, MZD+20, PKBZ20, RCM+22, SG22, TMH21, UBV+21]. **allyl** [DYK22, LWW20, MZ23]. **along** [SMMP+23]. **alpha** [sLLqX+23, MNWD20]. **alteration** [CP23]. **alterations** [JHH+22]. **alternation** [OR21]. **alternative** [ZHD+23]. **aluminides** [Pan22]. **Aluminum** [DYJ+22, FMM+23, LLW+21, RDMF21, SK20]. **Aluminum-nitrogen** [DYJ+22]. **always** [LFMG20]. **Alzheimer** [ZLH20a]. **Am** [LNC+23, WZL23]. **ambient** [ZWW+22]. **americium** [sLsHtW+23]. **amide** [BSS21]. **amidine** [HH23, UAH+20]. **amine** [MSM+20]. **amino** [HYY20, LC20, MZXL21, MBR21a, PPR21, SWML23, YLL+20, ZWL22]. **amino-ethyl-amino** [YLL+20]. **amino-substituted** [SWML23]. **aminolysis** [AAN+21]. **aminophosphoranes** [MFE+23]. **aminosalicylic** [TLT+22]. **Ammonia** [FGMO20, MSM+20, VSKG21, WCZ+20]. **ammonia-water** [WCZ+20]. **among** [MM21]. **amyloid** [ZLH20a]. **amyloid-** [ZLH20a]. **Analogies** [CRC21]. **analogous** [LPH22]. **analogs** [HLF23]. **analogue** [ABDD22]. **analogues** [PM20, ZLT+20]. **analyses** [CRGD+23, DC22]. **Analysis** [STN20, XBK+20, AAAAA23, AA20, BUKA21, BZW+21, BWLZ22, BRB+21,

BESG22, FAB+23, GN20, GMRKMCMC21, hHRN+23, JD20, KB23, KAA21, LSA+22, LS21, LPH22, LFMG20, NS22, NHNO20, Nat22, Ole21, OMA21, PVR20, PB23, Ram23, RNH23, SMCNH22, SP20a, TB22, OGT20, QDOC+21]. **Analytic** [NF20, RVK23, PJ20b]. **Analytical** [Fin21, TPCSD20, AB21, SC23]. **analyze** [Gun21]. **Analyzing** [DK21, WOE+22, AGK23, LG22, Rad21]. **anandamide** [CRGD+23]. **anatase** [RHS+21]. **anchored** [SDL+22]. **anchoring** [MZF21]. **Angular** [SDK+21, CSS+21]. **anharmonic** [TFF+22, WWF23]. **Anharmonicity** [MM22a, LNX+21, YXKJ21]. **anhydride** [WSSD21]. **ANI** [JLWH23]. **ANI-2x** [JLWH23]. **anilines** [LLQ+21]. **Anion** [LSOEAE22, THL+21, WWWC21, WYL22, ZZL+20a]. **anion-based** [THL+21]. **anions** [LCT+22, QdOdMC+21]. **anisotropic** [CZGW22, GUUG23, JS21, PASS21, WXHX22]. **Anisotropy** [YFX+22, GMRKMCMC21]. **annealing** [TSN+21]. **annihilation** [STT20]. **annular** [ZZXT21]. **annulation** [LZ21, YYL21, ZZZW20]. **anode** [EGLJQ+21, FMH+22, LFX+21]. **ansatz** [CFJ20, XgZX+22, BKB+23]. **antennas** [SFPH22]. **anthracene** [YZY+22]. **anthracenyl** [ZAB+23]. **anti** [APR20, HRA+22, LG21, TB22]. **anti-Covid** [TB22]. **anti-Hermitian** [HRA+22]. **anti-Markovnikov** [LG21]. **anticancer** [BSMI23, PSJ22]. **antiemetic** [hHNRA23]. **antifungal** [CS23, PB23]. **antimalarial** [SK21]. **antimonene** [MZF21, THL+21]. **antimony** [RGS23]. **antimony-oxide** [RGS23]. **antioxidant** [RGLG23, dPZFM+22]. **antioxidants** [dOSdASC+20]. **antiperovskites** [RKA+21]. **antiviral** [Bra21, KAA21, LAAP21]. **any** [GRFM20]. **any-particle** [GRFM20]. **apatite** [UV20]. **appearance** [GYC20, MM20]. **applicability** [RMWF20]. **Application** [DLZ+21, GN21a, KDY+22, MMP23, MT23, Rui22, dOSdASC+20, ZMJ+20, SSDF23]. **Applications** [RKI20, AMK+20, Ano22a, AIR+23, BT21, FZL+20, FMS+22, GSRG22, HBB+21, KHK+23, KM21b, LZSA20, LCX+21, Rac21, RP22, TMH21, WYZZ20, ZMOE23, ZG21, PSN23]. **applied** [HMBPJ+20, LRG+20]. **apply** [AS22]. **applying** [GZC21]. **approach** [BSMB23, EGLJQ+21, EAPCD20, HTNP21, HK22, Izs21, KKH21, KYL+20, KAG+20, MT23, PCEAG23, RKK+22, RSBK20, Roy20, SM22, SFT+21b, SS21, SG21, VL21]. **approaches** [AR22, CMM21, Kön21, SBM22]. **approximant** [BXWK22]. **Approximate** [PGROM20, P´23, TD22]. **approximation** [BA22a, GTV20, Hua20, NR21, PM22]. **approximations** [EB22, RKI20, VGSS20]. **aqua** [MGK23]. **aqueous** [BCLM+22, KK21, KLK21, LLW+21, SASA21]. **aqueous-phase** [SASA21]. **arbitrary** [GM21, WP22]. **arc** [ZHW23]. **arene** [BA21]. **arene-crown-** [BA21]. **arenes** [WLH+20, WHYL21]. **arising** [Dau23]. **arithmetic** [BDEM21]. **armchair** [MMP23]. **aromatic** [GMRKMCMC21, HRTSS+20, JS21, PGPHAPM20, Var23, YCSK20]. **Aromaticity** [PM20, APR20, LZZW23, SCZ21, SCAD+20, Tia21, ZFB+20]. **arrangement** [LC20]. **arrangements** [CZ21]. **Arsenene** [MZF21, HLL+23, HLZZ23, THL+21]. **arsenide** [NM23]. **artificial**

[AkAR+21, BSMI23, MSI22, WWL21]. **aryl** [KSPG23, TMX+22]. **arylation** [WSSD21]. **aryloxide** [MWCJ23]. **Asp** [BESG22]. **aspect** [MM20]. **aspects** [BUF+22, GNC20, HW21b, MP20]. **assembled** [PS22]. **Assessing** [FH21, ORL+20a, LCP21]. **Assessment** [Cha21b, KSP20, BGM+23, EB22, KRS+21, MK21, PVR20, TSHRS+20, YZD+20, ZYZ+22]. **assignment** [KMK21]. **assistant** [BHH20]. **assisted** [CWW+23, GKN+22, MJH+22]. **Asymmetric** [AA20, LLQ+21]. **asymptotic** [Yal23]. **asymptotics** [SSD22, SD23]. **asynchronous** [TXW+20]. **atmosphere** [LDS+23, YZD+20]. **Atmospheric** [LDS+23, CMM21, GHZ+23, LRG+20, MSS20, SP20a, SRS21, SYT+21, SXTZ23, XZGS23, ZZZ+20a, ZWZB23, YST+21]. **atom** [AR22, CRC21, CSL+23, CZJ+23, DG21, DLZ+21, HJL+23, HDF+21, KRK+21, LLX+23, LBG20, MF21a, SBA21, SLPS20, SPF+22, SPR21, ZGJ+20, ZZJ+23, ZHJ+20]. **atom-field** [CRC21]. **atom-supported** [LLX+23]. **Atomic** [AkAR+21, ÉC21, Gun21, MZD+20, BMF20, HMBPJ+20, HDF+21, Iri20, KAUB21, Lom21, MM20, RKK+22, RPT21a, RPT21b, SPF+22, SDK+21, SPR22, VP20, VL21, YCL+23]. **atomic-scale** [UBV+21]. **atomisation** [LCP21]. **Atomistic** [PP23, RBJ21, BCM23]. **atoms** [AA23, BPB+20, FK20, Fin21, GZWL22, HLF23, JVK22, JXM22, LT23, MR21, MAMB+22, NHNO20, Nan23, NZ20, RNFMC20, SJ20, SMMP+23, TAUM+23, TAMU+23, TT21a, WAM+20, WKH20, XJLH21, YÇDÖ21]. **atoms-in-molecules** [NHNO20]. **Atop** [KRB20]. **Atop-the-barrier** [KRB20]. **attractive** [GOR20]. **Aufbau** [TAUM+23]. **Augmented** [SY21, VP20]. **aurocarbons** [VNK+23]. **AuSi** [BCKN21]. **Automating** [QDOC+21]. **auxiliary** [SSS23]. **avoided** [SJ20]. **AzaBODIPY** [CCZ20]. **azirines** [LZ21]. **azobenzene** [CP23]. **azoles** [QLGZ23]. **Azure** [KLK21].

B [MZD+20, MBM+21, NG20, SLL+22, YFX+22, PGPHAPM20, APR20, CPL+21, ÉC21, GML+22, LMM+22, LFMF23, NHH22, RS23, SSIE20, SSIE21, WCM+23, ZFB+20, dPZFM+22]. **B-** [NHH22]. **B/N** [SSIE20]. **Ba** [Shi21, Tia21, XFW+20, VCM+21]. **back** [BSMI23, MSI22]. **back-propagation-artificial** [BSMI23, MSI22]. **backbone** [LFRTRP+20, ZZ22]. **Backflow** [NZ20]. **background** [SMCNH22]. **balance** [XWLZ20]. **band** [LMM+22, MBKA21, RK21, WWLL21, WLY+20]. **Bandgaps** [HZC21]. **bands** [KMK21]. **barrier** [ARRB+21, KV23, KRB20, KC23]. **barriers** [KV23, VKK+21]. **base** [GG20b, MHD20, VOK+20, WWWC21]. **base-promoted** [VOK+20]. **Based** [ZJW+21, AkAR+21, AAAAA23, AGK23, BVL22, BSS21, BCLM+22, CS23, CN21, CRKMC21, CSTD22, CSGR21, DSNZ+20, FFBH21, FZL+20, FWJ+23, GNC20, GMO+20, GPP+21, HLL20a, HRTSS+20, Hua20, hHNRA23, hHRN+23, JBPV21, JZL+21, JXL+21, JD20, KM23, KSPG23, KMH+20, KJA+21, KI20, KS21, LYT+20, LZ20, LAAP21, LMAA23, MSKA20, MGK23, MIM21, MJRS20, MA23, NG20, dRNS21, ORL+20a, PS22, PIA21, PLZT22, RRD+22, RKK+22, RNA22, RNB22, RNH23, RSD21, RR23, SIA20, SMCNH22, SK20, SMJ20, STN20, SWXM23, SSS23, SG20, SG21, STF21,

TSN+21, TB22, THL+21, TSS+23, TCX+22, WWL21, WZ20, WJL+21, XPZ20, XZ20, XWJ+21, ZZXT21, ZZ22, ZMS21, KHK+23, TCL+21, Üng23]. **bases** [RKG21, SE20]. **basic** [HW21b, LZL+21]. **basics** [Cla22]. **Basis** [Ale23, QdOdMC+21, BT23, DK21, GSMT+20, HMBPJ+20, KCM+23, LT23, RPT21a, STI20, SM22, SK21, SS21, TLL23, VP20, Var21]. **BaTiO** [ORL+20b, WXL+21]. **batteries** [EGLJQ+21, MZF21, MHS21, dRNS21, PSN23, ZYZ+22]. **battery** [FMH+22, LFX+21]. **BC** [MJA20, XHX+20, ZQZ+23b]. **B ==** [SLL+22]. **Be** [PCKP20, FGMO20, LL21, KDY+22, LWC+21, RMS+23, SKG23]. **bearing** [LLMQ20]. **Behavior** [PRC23, AAJ+23, DYZ+23, ISL+23, JSF+21, KHK+23, MWC+21, RMB+23, SG21, SLL+22]. **behaviors** [LDS+23, Üng23, XBL23]. **being** [KAA21]. **Benchmark** [KLT21, KAG+20, SK21, VKK+21, AMRS22, BHN23, TD22, TTTH20]. **Benchmarking** [Cha21a, GTC+23, Jan22, JLWH23, JS21, KK23b, PPCF+20, GZC21, KV23]. **benchmarks** [AIB21]. **benzamides** [ZZZW20]. **benzene** [hHRN+23, LSOEAE22, Mok21b, RNA22, RNB22, UP20, YXKJ21]. **benzenoid** [Kha23, LCX+21, RĐB+23, WYZZ20]. **benzoselenadiazole-pyrrole** [SCU21]. **benzothiadiazole** [SCU21]. **benzothiadiazole/benzoselenadiazole** [SCU21]. **benzothiadiazole/benzoselenadiazole-pyrrole** [SCU21]. **benzothiazole** [PPR21]. **benzoxazinone** [SSEI21]. **benzoxazole** [LLZ+20]. **berberine** [KK21]. **berkelium** [ASHPHCB20]. **beryllium** [Guh23]. **Bethe** [CFJ20]. **better** [TLL23]. **between** [ASO+22, AA23, CRC21, HLL20b, ID21, KZ21, KMK21, Kid21, LDS+23, MNN+20, MWBQ20, RGS23, Rad21, TSS+23, WXLL21, WCZ+20]. **beyond** [GTV20]. **BH** [fXmTlS+23]. **BH28** [KV23]. **Bi** [SBKT23, KM23, MAHRA+21, CZJ+23]. **bi-BN** [CZJ+23]. **bicyclic** [MSADA21]. **bilayer** [CPL+21, Mok21c]. **biliverdins** [MEBL22]. **binary** [BSMB23, Yan21]. **Binding** [MZXL21, MFC20a, CS23, CZ21, GRFM20, JXM22, LCH+22, WZL23]. **binuclear** [DTAS21]. **BiOBr** [GRZ+21]. **Biological** [MFJ+23]. **biopolymers** [BCLM+22]. **biphenyl** [BMH21]. **biphilicity** [MFE+23]. **bipyramidal** [VSKG21]. **bipyridyl** [ZQZ+23a]. **bis** [BSS21, KPTL23, LZS20, LNC+23, XWLZ20, XWJ+21]. **bis-1** [LNC+23]. **bis-amide-based** [BSS21]. **bismuthene** [MZF21]. **bispentalene** [ILPY+23]. **black** [GG20a, WTC+23]. **block** [CL21]. **Blockchain** [HHA23]. **blue** [CWL+22, DYJ+22, LYTS20, WLY+20, ZHFD+20]. **BN** [CZJ+23, ISL+23, Roy20]. **bodipy** [TPT20, HMA+22, MRI20]. **body** [Eti20, LBG20, RKI20, SMJ20, UP20]. **Bohm** [GN21b, KASAK23, WOE+22]. **Bohr** [JVK22]. **boiling** [HYHW22, LCX+21]. **Boltzmann** [BRF21, VL21]. **Bond** [BHN23, YXKJ21, AN20, AAN+21, APR20, CJVF+23, CPK22, HLL20b, JD20, KLT21, KAG+20, LAKJ20, LNX+21, LL21, LAAP21, LCY+23, ÖÇÖ21,

RR21, SMCNH22, SK20, SKG23, STF21, SLL+22, TTTH20, WLLS21, ZZF22]. **bonded** [AS22, MOB21]. **bonding** [ASO+22, AA23, CSY+21, DKK+20, KSP20, Kov20, LFRTRP+20, MZ23, NSM22, PCKP20, RNRBFC21, SFB20, VCM+21, XL22, ZWL22]. **bonds** [CLL20, LL21, PC22, SI20, VM20, WXLL21, ZL21]. **Book** [BRB+21, EM21, YST+21]. **boosts** [ZXS20]. **borane** [MSM+20]. **boride** [FMM+23]. **Born** [BA22a]. **boron** [CPL+21, MMP23, MCP+20, SZMM22, THS20]. **boroxol** [ZFB+20]. **boroxol-type** [ZFB+20]. **borylation** [TMX+22]. **Bose** [PMdN21]. **both** [QDC+22]. **bottom** [LC20]. **bottom-up** [LC20]. **Bound** [Yal23, PGROM20]. **boundary** [LLC20, PP23]. **Bounds** [RA20, CDR20, RMWF20]. **Box** [GSMT+20]. **Br** [AMK+20, AMM21, GSRG22, PAS+21, RKA+21]. **branching** [CL22]. **Braun** [CBK+20]. **Braun-like** [CBK+20]. **BrCl** [WAW+21]. **Brezovnik** [Ano22a]. **bridge** [CZW21, HFF22]. **bridge-state** [CZW21]. **bridged** [LTC+23, SSIE21, SSS23, XWLZ20]. **bridges** [LYT+20, SE22]. **bridging** [JHH+22, MZ23]. **bright** [DSNZ+20]. **broadening** [UP20]. **bromanes** [NHNO20]. **bromochloroethane** [WAW+21]. **Building** [MNN+20]. **bulk** [LHL+21, MHD20, RC20, XHS+23, Yan20]. **butadiene** [BTS+21, SRS21]. **butene** [WWZ+20, YHW+22]. **butyl** [CMM+22]. **butyric** [LMAA23]. **BX** [PVR20]. **Bypassing** [JJJM21]. **byproducts** [ZHD+23].

C [Ari21, CSL+23, EB22, GMRKMCMC21, ILPY+23, LWH+21, LZZ+20, SK21, SBAT23, SRS21, TWT+21, ASO+22, ABDD22, Cha21a, CYL+23, CCZ20, DFK20, ÉC21, GMO+20, GMRKMCMC21, HL20, JSF+21, KAG+20, LWC+21, LWR21, LFMF23, MZ21, MOB21, NZ20, NTND23, QDJY23, RS21, RS23, RINHY20, SSK20, STF21, VNK+23, WSSD21, WWKH22, WHYL21, WAW+21, XL22, YCPW20, YCSK20, ZHG+22, ZWZB23, SMCNH22]. **c-DFT** [SMCNH22]. **C-H** [WHYL21]. **C-Mg** [KAG+20]. **C-NMR** [GMRKMCMC21]. **C40** [Pan20]. **C61** [LMAA23]. **Ca** [PZGH+20, Tia21, XFW+20, RMS+23, WY20]. **CaCl** [WY20]. **cadmium** [FCL22]. **CaF** [HNO+21]. **caffeine** [KVCS21]. **cage** [AJC+21, ELH20, GMO+20, PRC23, TWT+21, dPZFM+22]. **cage-like** [AJC+21]. **cages** [GW21, GZWL22]. **calcium** [ZLH+20b]. **calculating** [Cio22, Izs21]. **Calculation** [FCL22, LNE+20, NZAH21, AKKN20, EB22, Eti20, GM21, KRS+21, sLLqX+20, QLGZ23, SAP22, STT20, TCX+22, WP22, XJLH21, ZS21]. **Calculations** [Cha21a, GRFM20, BCKN21, BBAA21, BVL22, BCM23, CSL+23, CN21, CRKMC21, CXZ+21, GMO+20, GRZ+21, GUUG23, HK22, HMN20, HCZ20, JXM22, Kan22, KC23, LRG+20, LCH+22, LWH+21, MKD21, MP20, OGT20, OAJ21, ORL+20b, PL20, QdOdMC+21, QOM+20, Rac21, SBA21, SK21, THS20, UR23, VNK+23, WZ20, Wan21, XFW+20, Yal23, ZRR+21, ZGJ+20, ZYZ+21b, ZLH+20b]. **calculus** [NdVVT22, TVdVN21, TVdVN22]. **Calibration** [GKPK21]. **calix** [BA21].

Can [FGMO20, KM21a, LL21, Var23]. **cancer** [Hav21, MA23]. **canonic** [SM22]. **Canonical** [Var21]. **capability** [RGLG23, ZHW23]. **capacitance** [CLLC21, RBJ23, SUG20, XWS+22, YCL+23]. **capacities** [YHW+23]. **capacity** [END+23, LFX+21, MNN+20, ZHG+22]. **capped** [JHH+22]. **capture** [DRV20, Kan21, Kan22, RS23]. **Capturing** [RF23]. **carbamido** [EM21]. **carbazole** [LK20, MSKA20]. **carbazole-based** [MSKA20]. **carbene** [DDSB22, JRA21, KZ21, LLZ+20, LLMQ20, PM20]. **carbene-catalyzed** [JRA21, LLZ+20]. **carbide** [FMH+22, JSF+21, MKKK22]. **carbocation** [VdM22]. **Carbon** [KS21, AAN+21, AKKN20, Ali20, AA20, EGLJQ+21, GW21, GG20a, HLL20a, Jah20, KWWZ20, KOB20, KS23, LQZ+21, NS22, PNC20, SUSS23, THS20, TT21a, XL22, ZMS21]. **carbonate** [ASHPHCB20, ZLH+20b]. **carbonated** [UV20]. **carbonates** [LLLL20]. **carbons** [ILPY+23, KS23]. **Carbonyl** [KBR+20, LZL+21, MSM+20]. **carboxylate** [LLW+21]. **care** [RBSW21b]. **career** [SF20b]. **Carlo** [HZC21, KA23, NZ20, SRH20, SS21]. **carrier** [Dau21, WWLL21]. **carrier-envelope** [Dau21]. **carriers** [RSM+22]. **Case** [HMN20, Ari21, INV22b, MM20, NHNO20, NTND23, PCEAG23, Var23, YCSK20]. **cases** [RRSF22]. **CASPT2** [AMRS22, BCKN21, VNK+23]. **CASSCF** [BCKN21, AMRS22, CN21]. **catalysis** [HYY20, PGÁML21, SRH20]. **catalyst** [AKKN20, GKK21, LK21, Roy20, SDL+22, VKS21, WLP+20]. **catalysts** [AR22, CSL+23, DLZ+21, GKPK21, KS21, LLX+23, LZL+21, RSD21, WWM+22, fXmTlS+23]. **Catalytic** [GOS20, AKKN20, ES21, KS23, LZL+21, SE20, fXmTlS+23]. **catalyzed** [CYJC20, CSY+21, JRA21, LLZ+20, LZ21, LG21, LWR21, QDJY23, SLdS20, TXW+20, WWZ+21, WSSD21, WLH+20, YZD+21, YYL21, ZZZW20, CMM+22]. **catalyzing** [WWM+22]. **caterpillars** [Ye20]. **cathode** [KM21a, MHS21]. **cation** [DTAS21, GTAL23, Iri21, MKD21, Mka20]. **cation-circumcoronene** [GTAL23]. **cationic** [DTAS21]. **cations** [BCM+22, CYJC20, ELH20, KKH21, KML23, PCKP20]. **cavity** [BUF+22, YÇDÖ21]. **cavity-induced** [BUF+22]. **CC2** [JS21, JS21]. **CC3** [JS21]. **CCSD** [JS21, BT23, JS21, VNK+23]. **CCSDfor** [TD22]. **Cd** [WXHX22]. **Ce** [SMK+23]. **Celebrating** [KKRR21]. **cell** [MSKA20, ZZZ+23, SSS23]. **Cellmetry** [PS23a, PS23b]. **cells** [BSS21, FFBH21, FZL+20, KPMAB22, KMH+20, KJA+21, LZ20, MJH+22, PIA21, PGPHAPM20, PSJ23, SIA20]. **Center** [GM21]. **centered** [DKK+20, SF20a]. **centers** [SCAD+20]. **central** [BA22a, Nat22]. **cephalosporins** [KLT21]. **ceramics** [PL20, XFW+20]. **cerium** [sLhZX+22]. **Cernusák** [LUB23]. **certain** [AGK23, LAAP21, RRSF22]. **CF** [CLLC21, LDS+23, LZL+21, TCX+22, YZL+21b, YHZ+22]. **CF3** [HMN20]. **CFCN** [LDS+23]. **CH** [HMN20, ZHS21, ASO+22, BZP+20, CZC+23, WWZ+21, ZZZ+20a, ZHS21]. **Chain** [DYK22, AII21, CLC+21, KSPG23, LC20, LSG21, LGW23, MAK+22]. **chain-initiation** [CLC+21]. **chains** [BMR21, FYL21, ZZXT21]. **chalcogen** [CLL20, ZLT+20]. **chalcogenides** [LYW+20]. **chalcones** [ZAB+23].

Challenges [SC21, GG22, ZG21]. **change** [RNRBFC21]. **channel** [TSHRS+20]. **character** [GMRKMCMC21, JJJM21]. **Characteristic** [CRKMC21]. **characteristics** [CXZ+21, LFRTRP+20, SFB20, SCY+23, fXmTlS+23, XHX+20]. **Characterization** [JD20, AKK+21, RPAA22]. **Charge** [KVCS21, ABS20, BZW+20, BS20, FK20, Gun21, KKK23, MKM+20, Mok21c, RR21, SCZ21, Üng20, VL21, XAM+22, YCPW20]. **charged** [KKH21]. **CHCl** [HMN20]. **chelotropic** [SMMP+23]. **Chem** [GM21, Sur22]. **Chemical** [Cha21a, RMWF20, WFG+21, ZWZB23, ADZA21, APR20, AD22, BDEM21, BPB+20, CFJ20, CLW21, DAR+21, FYL21, GB21, GZC21, GG20a, GMRKMCMC21, HMN20, HCZ20, IAI20, LC20, LRG+20, LFRTRP+20, LL20, LCX+21, LDS+23, MJA20, MJH+22, MB23, MSI22, NSM22, PCKP20, RRS21, RNB22, SMN+23, SM22, SBM22, SK21, SBKT23, SMS23, Sta21, VKS21, VOK+20, ZG21, ZHW23, ZZF22]. **chemicals** [GG20b]. **chemist** [RBSW21b]. **Chemistry** [KKRR21, BHH20, BWR22, Cio22, EPMC20, GTC+23, HHA23, HHG+21, KBR+20, KS22, MFK22, MJRS20, Mos21, PGÁML21, RP22, Sha20, Shi20, VN21, WWL21, HHG+21]. **chemists** [Cla22]. **chemodivergent** [ZZZW20]. **chemosensor** [HRTSS+20, TSHRS+20]. **chiral** [ZLG22]. **Chirality** [XAM+22, LNX+21, NYX+22]. **Chirality-helicity** [XAM+22]. **chitosan** [SU22]. **chloride** [DYK22]. **chlorine** [SRS21]. **chlorophylls** [SIA21]. **CHO** [ZHS21]. **chromophores** [GA20, SFB20]. **CHZ** [WDS+20]. **CIE** [Jan22]. **cigar** [PMdN21]. **cigar-shaped** [PMdN21]. **circuit** [YZW+23]. **circular** [RG20]. **circumcoronene** [GTAL23]. **cis** [WWZ+20, Mka20]. **cis-1** [WWZ+20]. **Cisplatin** [ZYZ+21a]. **Cl** [AMK+20, AMM21, MZ23, PAS+21, PVR20, RKA+21, CYL+23, GNC20, MZ23, SGWW22, SCY+23]. **Clar** [RRD+22]. **Clar-structure-based** [RRD+22]. **class** [LPH22, PMGR+21]. **Classical** [RRSF22, BM21, DG21]. **classically** [FGMO20]. **cleavage** [KAG+20]. **ClO** [WDS+20, FWJ+23, WDS+20]. **cloud** [RBSW21b]. **cluster** [AIB21, BBTN23, BBG20, Cha21b, FK20, GDR21, Gun21, HTNP21, Hua20, JBPV21, KBR+20, Roy20, SGWW22, Var21, WWF23, XgZX+22, ZFB+20, ZG21]. **clusters** [AJC+21, APR20, BTS+21, DCY21, GNC20, GYC20, HFL23, JZL+21, JLWH23, KYL+20, LAKJ20, LDK23, MFC20a, MOB21, NLA+21, PPCF+20, RGS23, RMB+23, SSDF23, SBJ20, TSS+23, TT21b, ÜB20, WYL22, Yan21, ZZZ20b]. **Cm** [WZL23]. **Cmcm** [PP21]. **Cmcm-Mo** [PP21]. **CN** [PVR20]. **CNT** [SUG20]. **CO** [KWWZ20, LLZC20, XWS+22, YCL+23, DYJ+22, DRV20, DK21, ER22, HLL20b, Kan21, LLLL20, LXWZ21, MZ23, NHH22, QdOdMC+21, RINHY20, SSIE20, SSEI21, SSIE21, WOE+22, LQZ+21, MZD+20, MHG+23]. **co-doping** [DYJ+22]. **coal** [ZL23]. **coatings** [ARRB+21]. **cobalt** [RMB+23, SG21, SP20b, fXmTlS+23]. **cobalt-based** [SG21]. **cobalt-phosphorus** [RMB+23]. **codoped** [KS23]. **coefficient** [KRS+21]. **coefficients** [HYHW22, UR23]. **CoF** [SP20b]. **coherent** [Dau23]. **CoI** [MKM+20]. **coindices** [DAR+21, SUSS23]. **cold** [KK23a]. **Collaboration**

[GOR20, MNN+20]. **collision** [CLS+22]. **color** [Jan22]. **CoM** [SU22]. **CoM-polynomial** [SU22]. **combined** [DYJ+22, GNC20, sLsHtW+23, NF20, STI20, YHZ+22, ZKP22]. **Combining** [FWY+22, dOSdASC+20, YHW+23]. **coming** [RPT21b]. **Comment** [Cin20, MMM20, MAK+22, NACP21, TdV21, OB21a, OO21b]. **Compact** [WP22, NdVVT22, TVdVN21, TVdVN22]. **Comparative** [BSMI23, JWZZ20, Kha23, Ole21, SU22, AB21, CYL+23, HTNP21, HLF23, HFL23, NS22, dLRdLJ+20]. **compared** [NYX+22]. **Comparison** [CLL20, SLL+22, AIB21, BT23, GSMT+20, HFF22]. **competing** [WZL23]. **Competition** [WCZ+20]. **complete** [BT23, HP21, Var21]. **complete-basis-set** [Var21]. **completeness** [Sha20]. **Complex** [BAM20, UBW+22, JBPV21, KDY+22, Kön21, LTC+23, RR23, SBAT23]. **complexes** [ASHPHCB20, AS22, CYJC20, DSNZ+20, EB22, GTAL23, Kov20, KPTL23, LLW+21, LSOEAE22, LLMQ20, MFJ+23, MGK23, MZ23, dAOdASP+20, PPR21, PLT+20, PS23b, RR21, RKG21, SFPH22, SP20a, SBKT23, Shi21, SN21, SLL+22, Üng23, VGSS20, VSKG21, WXLL21, ZQZ+23a]. **complexity** [EAPCD20, EAPCD21, FLZP23, GN21b, Nat22, SSD22]. **complexity-like** [SSD22]. **compliance** [MM22a]. **component** [AMM21]. **composite** [HYC+21, KV23, LMAA23, SBA21, SUG20, VKK+21]. **composites** [EGLJQ+21, KAUB21]. **compound** [FGW+22, GTC+23, HNO+21, sLLqX+20, LHL+21, ONH+21, WXHX22]. **compounds** [AN20, AMK+20, BRHECY+22, BBAA21, HBB+21, HRTSS+20, KLRS22, LAAP21, MSM+20, MBM+21, QLGZ23, QDJY23, SK21, dOSdASC+20, SG21, SYD+23, WCM+23, XL22, XWLZ20, XWJ+21, Yan20, ZRR+21]. **comprehensive** [Eti20, RCM+22]. **compressed** [SBA21]. **comprising** [PC22]. **Computation** [AIAG21, CDG+21, MSA22, TCSG+20, Boz21, RR23]. **Computation-driven** [CDG+21]. **Computational** [AAN+21, ABDD22, BZW+21, CLL23, GHZ+23, GMRKMCMC21, ISL+23, JHH+22, KI20, KKRR21, LWR21, RGLG23, RYC+20, SBG21, TMX+22, VSKG21, WJL+21, ZJW+21, ZZZW20, BY23, BHH20, BSS21, BRB+21, CMM+22, EPMC20, GKPK21, GKK21, GG22, HFL23, KBR+20, KDM+22, MZF21, MNN+20, ÖÇÖ21, RCM+22, RBSW21b, SNL+23, Shi20, Shi21, SCU21, TCSG+20, UBV+21, WLH+20, WHYL21]. **Computationally** [JRA21, RF23]. **computations** [WWF23, AIR+23]. **computed** [BBG20]. **Computing** [LG22, NS22, Ano22a, AKP22, BT21, Cla22, KCM+23, LSG21, RBSW21b]. **CoNbMnZ** [SG22]. **concentration** [CMGH+21, WWLL21]. **concept** [SSIE20, Var23]. **conceptual** [PCEAG23]. **concerted** [TXW+20, WAW+21]. **condensates** [PMdN21]. **condensed** [RKI20]. **condensed-phase** [RKI20]. **condition** [SMN+23]. **conditions** [ISL+23, Sør21, ZWW+22]. **conductance** [BMH21]. **conductivity** [LYPD23, SYD+23, UBW+22, YFX+22].

configuration [ATL+20, BZW+20, dSFdSdMdM20, GOT+23, sLsHtW+23, MKD21, SPR21, SPR22, UR23, ZGJ+20, ZS21, dLRdLJ+20]. **configuration-interaction** [ZGJ+20]. **configured** [ZMS21]. **confined** [BBTN23, EAPCD20, EAPCD21, HJL+23, LBG20, MR21, SJ20, SLPS20, TAMU+23, YÇDÖ21, ZZJ+23, ZHJ+20]. **confinement** [CP23, ISL+23, RNFMC20, RNRBFC21]. **conformation** [WV21]. **Conformational** [BT23, BZW+21, BWLZ22, BESG22, HYY20, MBR21a, ZGCF20]. **conformer** [FH21]. **conformers** [CRGD+23]. **conical** [WAM+20]. **conjugate** [KRB20]. **Conjugated** [KOB20, HFF22, KZ21, KK23a, LYT+20, OR21, SSIE21, ZIA20]. **Conjugated-carbon** [KOB20]. **conjugates** [MA23]. **conjugation** [ZZ22]. **connection** [TAMU+23]. **connective** [WYZZ20]. **connectivity** [GW21]. **consistent** [HK22, HP21, SM22, VGSS20]. **consortium** [MNN+20, Shi20]. **constant** [LHL+21]. **constants** [BESG22, HYHW22, JAZ+20, MM22a, OAJ21, PS23b, YZW+23]. **Constraint** [AAAAA23]. **Constraint-based** [AAAAA23]. **construct** [LWR21]. **Constructing** [TPB+20]. **Construction** [ZMOE23]. **contact** [VdM22]. **contained** [Eti20, LXZ+21a]. **containing** [AN20, BSMB23, HYC+21, SSEI21, TTTH20]. **content** [GZWL22]. **continuation** [LBP20]. **Continuum** [BVL22]. **contracted** [HRA+22]. **contributions** [RĐB+23]. **Control** [LNX+21, Dau23, DSNZ+20]. **Controllable** [GKN+22]. **Controlling** [Dau21, GZCY22]. **convergence** [BBG20]. **conversion** [BTS+21, Kan21, LLZ+20, RINHY20, SIA21]. **Conversions** [TWT+21]. **Cooperative** [WXLL21, ZL21]. **cooperativity** [MOB21, LL21]. **coordinate** [Tak22a, Tak22b]. **coordinated** [MSOA23]. **coordinates** [Bra21, MM22a]. **coordination** [MZ23, SCAD+20, HLF23]. **coplanar** [WJL+21, XWJ+21]. **copolymers** [BSS21, SCU21]. **copper** [LTC+23, SDK+21, ZPS+20]. **core** [GTAL23, JHH+22, JXM22, KMH+20, LNE+20, MZT20, ZMOE23]. **core-level** [LNE+20]. **CoRhZrZ** [LMM+22]. **corona** [AGK23, LS21]. **coronene** [HAA+23]. **coronoid** [CSGR21]. **correct** [CN21]. **corrected** [EB22, GMO+20]. **Correcting** [CM21]. **correction** [BSH+21, KA23]. **corrections** [AMM21, Iri20, Iri21, Nan23, XJLH21]. **correlated** [BBTN23, CPK22, JIFM22, SPR21, SPR22, Var21, WWF23]. **correlation** [ATL+20, AA23, Hua20, sLLqX+23, PT21, SP20b, STT20, VP20, ZIA20, ZS21]. **correlation-polarization** [STT20]. **correlations** [LTC+23]. **Corrigendum** [Ano21a, GM21, SDS20]. **corrolazine** [WWZ+21]. **corrosion** [UBV+21]. **CoSi** [ONH+21]. **cost** [KV23, KAG+20, TCSG+20, VKK+21]. **cost-effective** [KV23, KAG+20]. **Coulomb** [Dau21, HJL+23, MF21a, WWKH22, XJLH21]. **counting** [Pev21]. **coupled** [AIB21, BBTN23, BBG20, CDD23, GDR21, HTNP21, JBPV21, Roy20, SGWW22, SY21, Var21, WWF23, Xav23, XgZX+22]. **coupled-cluster** [AIB21, BBTN23, BBG20, HTNP21, SGWW22]. **couplers** [KA21]. **coupling**

[AAM+20, BESG22, JAZ+20, KWWZ20, LLLL20, MKD21, OR21, UR23, WLH+20, YYL21, ZS21, ZPS+20]. **covalency** [ASHPHCB20]. **covalent** [HW21a, MC22, MFK22, TCSG+20]. **Cover** [Ano20a, Ano20l, Ano20p, Ano20q, Ano20r, Ano20s, Ano20t, Ano20u, Ano20v, Ano20b, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20m, Ano20n, Ano20o, Ano21b, Ano21q, Ano21r, Ano21s, Ano21t, Ano21c, Ano21d, Ano21e, Ano21f, Ano21g, Ano21h, Ano21i, Ano21j, Ano21k, Ano21l, Ano21m, Ano21n, Ano21o, Ano21p, HOVG20a, INV22a, MBR21b, MM22b, RBSW21a, SFT+21a, WV20a]. **coverage** [DB20]. **COVID** [KAA21, LAAP21, RNH23, TB22]. **COVID-19** [KAA21, LAAP21, RNH23]. **CoZr** [TMH21]. **Cp** [MZ23]. **Cr** [ARRB+21, LLMQ20, MZ23, YZD+21]. **Cr/PNP** [YZD+21]. **Cr/PNP-catalyzed** [YZD+21]. **Crámer** [EAPCD21]. **criteria** [Pev21]. **Critical** [SDS19, BGM+23, HZZZ22, SDK+21, SDL+23, SDS20]. **cross** [KMH+20, MW21, ZHD+23]. **cross-linking** [ZHD+23]. **crossing** [KWWZ20, LYTS20, SV21, SJ20, TPB+20]. **crossover** [KGSD20, KPTL23]. **crotonaldehyde** [CMM21]. **crown** [BA21, TT21a]. **CrSi** [Pan20]. **crude** [BXWK22]. **crystal** [BRB+21]. **crystallization** [TAS21]. **crystallography** [MM22c]. **Cs** [BA21, RSM+22, ZCL+22, ZQZ+23b]. **CsSnI** [MT23]. **CsTmCl** [AAM+20]. **CTDE** [YZD+20]. **Cu** [LYW+20, MHS21, OMA21, Yan20, BWBR21, CZGW22, DB20, GZWL22, KM23, LYPD23, SBJ20, TXW+20, fXmTlS+23, XL22]. **Cu-porphyrazines** [BWBR21]. **CUAGAU** [Cha21b]. **CUAGAU-2** [Cha21b]. **Cuban** [GG22]. **cubic** [AGK23, ACM20, XFW+20]. **cuboidal** [PPCF+20]. **cucurbit** [MZXL21, MGK23, MI20, PSJ22]. **cumene** [CLC+21]. **cumulenes** [XAM+22]. **Curie** [SMP23b]. **Curl** [SMN+23]. **current** [PM20, SIA21]. **Curtius** [LFMG20]. **curve** [Kid21, LSA+22]. **curves** [TFF+22]. **cusp** [Cio22, JIFM22]. **customization** [Ale23]. **cut** [Ano22a, BT21]. **cyanic** [ZLT+20]. **cyanobenzene** [KJA+21]. **cyclic** [LFRTRP+20, Rad21]. **cyclic-triphosphazene** [LFRTRP+20]. **cyclization** [QDJY23, YCSK20]. **cyclo** [JJJM21, WWWC21]. **cyclo-N** [WWWC21]. **cycloaddition** [KZ21, MSADA21, PPCF+20, SBM22, TXW+20]. **cyclobutene** [MAMB+22]. **cyclodextrin** [BSH+21]. **cyclodextrins** [BRHECY+22]. **cyclohexanedione** [MOB21]. **cyclohexylamine** [MFJ+23]. **cyclooctane** [LGW23]. **cyclooctatetraene** [CMY22]. **cycloparaphenylenes** [ZQZ+23a]. **cyclopentadiene** [ASO+22, PVR20]. **cyclopentano** [MI20]. **cyclopentano-cucurbit** [MI20]. **cyclopropanol** [LWR21]. **cylinder** [FLZP23, QSZ23]. **cylinder-nonorientable** [QSZ23]. **cytidine** [SE22]. **cytochrome** [QDJY23]. **cytosine** [Ram23, SE22, UIIP23].

D [GXL+22, GMRKMCMC21, JWZZ20, JS21, Mka20, XPZ20, ZZXT21, DKK+20, GRLH21, GMRKMCMC21, JHH+22, MKKA21, PGPHAPM20, PCKP20, UHK+22, XPZ20]. **D-A** [JHH+22]. **D18** [ZZZ+23]. **D8** [PP21]. **dark** [DSNZ+20]. **Data** [OGT20, GTC+23]. **database**

[KV23, MJH+22, TTTH20]. **DCCnT** [XZ20]. **deactivator** [FMG23]. **DEAL** [KKRR21]. **deamination** [UAH+20, UIIP23]. **Debye** [WWKH22, WCM+23]. **decay** [SV21, TSHRS+20]. **deciphering** [Var23]. **decomposition** [AIB21, BWLZ22, CYL+23, CMM+22, HCZ20, Hua20, LZL+23, MWC+21, SWXM23, SDL+22, TCX+22, WWZ+20, YHZ+22]. **decorated** [MJA20, RS21, ZHG+22]. **decoration** [QDC+22]. **Deep** [LACP21]. **deeper** [ZYZ+21a]. **defect** [CLLC21]. **defected** [AKKN20]. **defective** [HLZZ23, LK21]. **defects** [QDC+22, RMM+22, SPF+22]. **deficient** [LZ20, SBKT23]. **defined** [RKI20, Tak22a, Tak22b]. **definitions** [CPK22]. **deformation** [AA20, MNWD20]. **Deformations** [BRHECY+22]. **deformed** [PGROM20]. **degeneracies** [BUF+22, ZZJ+23]. **degenerate** [Xav23]. **degradation** [CXZ+21, SRS21, SYT+21, ZWZB23]. **Degree** [MA23, SSD22, AGK23, CSGR21, hHNRA23, hHRN+23, PS22, RNA22, RNB22, RMWF20, RR23, SF20b, TB22, Wan21]. **Degree-based** [MA23, hHNRA23, RNA22, TB22]. **dehydrogenation** [DB20]. **delayed** [SYL+21]. **delimited** [BVT20]. **delivery** [PSJ22]. **delocalization** [Rad21]. **dendrimers** [MSA22]. **Deng** [NR21]. **dense** [CLS+22]. **densities** [LBG20]. **Density** [AMRS22, BA21, CXZ+21, DRV20, DPC+20, KRS+21, MR21, OKK+22, RBJ23, SPF+22, Shi21, SBJ20, Tak22b, VGSS20, XWS+22, dPZFM+22, AAYA23, ATL+20, AAAAA23, AA20, ABDD22, ARRB+21, BY23, BBAA21, BZP+20, BMH21, BRB+21, BB20, Boz21, BSH+21, CPL+21, Cio22, DFK20, DS20, EGLJQ+21, EB22, Eti20, FFBH21, FMM+23, GMO+20, GTV20, HMBPJ+20, Höf21, HW21a, Hua20, Jan22, JMOW20, JZL+21, KZ21, KPMAB22, KVCS21, KYL+20, KAG+20, KH20, KS23, LT23, LLW+21, LK21, sLsHtW+23, LLX+23, LCP21, LSS+21, LDS+23, LFMG20, MSKA20, MKKK22, MZ21, MSADA21, MIM21, MOB21, MB23, MPBL23, MP20, MHG+23, Nag20b, Nag22, OAJ21, PM22, PJ20b, Pev21, PCEAG23, PRC23, QdOdMC+21, QOM+20, RSD21, RPT21b, RVK23, SAP22, SK20, SMJ20, STN20, SK21, SF20a, SSS23, SG20]. **density** [STF21, Tak22a, TXW+20, THL+21, TSS+23, TCX+22, TT21b, WZ20, XAM+22, XZ20, XWLZ20, XQJ+21, YHW+23, YZD+21, ZJW+21, ZZZ+20a, ZZLC20, ZXS21, ZYZ+22, ZHG+22, ZZXT21, BVL22, PD22, SSEI21, TEEH23]. **density-density** [DS20]. **density-fitted** [Boz21]. **density-functional** [LDS+23, STN20, SF20a]. **density-to-potential** [KH20]. **dentate** [WZL23]. **deoxycytidine** [SE22]. **dependence** [BS20, BWLZ22, CLL20, ORL+20b, ZGJ+20]. **dependent** [BUKA21, BMF20, Dau21, GTC+23, HW21b, HYHW22, Jan22, KVCS21, sLhZX+22, sLLqX+23, LHL+21, MSKA20, MBKA21, MSCM23, NACP21, OO21a, OO21b, PM22, QFA+23, SAP22, STN20, UBW+22, WZ20, XZ20, ZZLC20]. **dephasing** [CZW21]. **deposition** [LQZ+21]. **depth** [YHW+22]. **Depurated** [Cin20, MMM16, MMM20]. **derivation** [Eti20]. **derivative** [HTNP21, ILPY+23, LYT+20, LZ20, LG22, MVF+23, TPT20, ZWW+22, dPZFM+22]. **derivative-based** [LYT+20, LZ20]. **derivatives** [BSMI23, Boz21, FSR+22, GXL+22, hHRN+23, JXL+21, KML23, LL20,

LPH22, LSOEAE22, MZ21, MSI22, NF20, NIA21, NTND23, PCEAG23, RNA22, RNB22, RGLG23, SSEI21, SFPH22, SBM22, SWML23, SU22, SRS21, UAH+20, WXLL21, ZJW+21]. **derivatives-A** [NTND23]. **derived** [Bra21, XAM+22]. **described** [FGMO20]. **descriptors** [BSMB23, Hao21, HZZZ22, IMJ21b, JPSC20, KSM+23, RSD21, RC20, SMMP+23, SZMM22, WWL21, WWLL21, YZW+23]. **Design** [PVR20, FZL+20, FAJOF20, JXL+21, LZ23, MFK22, RGLG23, SUG20, VN21, WJL+21, XWLZ20, XHS+23, ZZXT21]. **designed** [FGW+22, TSN+21]. **Designing** [KMH+20, KJA+21, XZ20, KPMAB22, SSIE21, SCU21]. **desorption** [FK20]. **detachment** [KRA+23, TSN+21]. **Detailed** [UBV+21]. **details** [MP20]. **detecting** [LZ23]. **determination** [ATL+20, HLL20a, PS23a, PS23b]. **determining** [SP20a]. **Deterministic** [BRF21]. **detonation** [LL20]. **deuterium** [STI20]. **Development** [CLS+22, Tak22a, Tak22b, Cha21b, dOSdASC+20]. **device** [KM21b]. **devices** [AAJ+23, KHH+21, MTA+22, SG22]. **devil** [MP20]. **DFT** [AAYA23, AIR+23, CRKMC21, CMM21, Cha21a, Cha21b, GZC21, GNC20, GRZ+21, GUUG23, HMA+22, HMN20, KLRS22, KHK+23, KLK21, KPTL23, KC23, LLLL20, LZ21, MKKA21, MGK23, MZ23, MEBL22, Mka20, MT21, MT23, PGPHAPM20, PVR20, PPCF+20, PLZT22, Rac21, RMS+23, RS23, RKI20, SMCNH22, SMP23a, SKR+21, WYL22, XZ20, ZAB+23, ZKP22, ZZZ20b]. **DFT-based** [KHK+23]. **DFT-in-DFT** [RKI20]. **DFT/GIAO** [GZC21]. **DFT/periodic** [PGPHAPM20]. **DFTB** [NLA+21]. **DH** [TCSG+20]. **DH-SVPD** [TCSG+20]. **di-superatomic** [Yan21]. **diabatic** [MKD21]. **diagonal** [Cio22]. **diamide** [RED21]. **diamond** [HW21a, INEB23, PP23]. **diamondoid** [STF21]. **diarylethenes** [NYX+21]. **diatomic** [AB21, BA22b, CJVF+23, FWY+22, HSV22, HTNP21, KASAK23, WOE+22, XJ20]. **diborane** [DKK+20, LSOEAE22]. **diborene** [SLL+22]. **dichroism** [RG20]. **dicyclobutadieno** [LG22]. **dielectric** [BPB+20, HYHW22, YZW+23, ZHW23]. **Diels** [ABDD22]. **difference** [VL21]. **different** [CLL20, GZC21, GZCY22, JZX+20, MEBL22, NLA+21, PRC23, Rad21, RR21, Üng20, VL21, WZ21, WZL23, XZ20, ZZ22]. **Differentiation** [CLW21]. **diffuse** [VP20]. **diffusion** [HYHW22, HZC21, KC23, ZL23]. **difluoro** [CMM21]. **difunctionalization** [AAN+21]. **dihalogen** [AMM21]. **diiodocyclododecanes** [MF21b]. **diketone** [LWR21]. **diketones** [RKG21]. **dilute** [MMP23]. **dimensional** [BFW+22, CZJ+23, DLZ+21, EAPCD20, EAPCD21, HAA+23, KMH+20, LHZG23, LLX+23, LZZW23, dRNS21, Ole20, Ole21, PMGR+21, RYC+20, SAP22, SZMM22, SCY+23, SYZF22, XQJ+21, YZY+22]. **dimer** [FAX+23, Guh23, MYS23, RNRBFC21, SFB20]. **dimeric** [ZPS+20]. **dimerization** [CMY22, GOS20, HYHW22]. **dimers** [LK20, ZLT+20]. **dimethyl** [KMK21]. **dimethylaminophenyl** [BRB+21]. **dimethylcyclohex** [BRB+21]. **dimethylcyclohexane** [BZW+21]. **dimethylcyclohexyl** [BWLZ22]. **dinitrogen** [Kov20]. **dinuclear** [LTC+23]. **diode** [Üng23].

diodes [LK20]. **dione** [LZS20]. **dioxide** [GG20a, HLL20a, KWWZ20, LSA+22]. **dioxin** [ARBM21]. **dioxin-like** [ARBM21]. **dioxopyrimidine** [BY23]. **dioxygen** [DTAS21]. **Dipole** [WWKH22, ACM20, BCM+22, CZ21, HTNP21]. **Dirac** [CRC21, KASAK23]. **direct** [WLY+20]. **directed** [WSSD21]. **Dirichlet** [Ole20, Ole21]. **Discerning** [MAMB+22]. **discovery** [GKK21, HBY20]. **discrepancy** [ID21]. **discrete** [TPCSD20]. **discussion** [Nan23, Yos20]. **disease** [ZLH20a]. **diseases** [PB23]. **dislocation** [BU20]. **dispersion** [BSH+21, GMO+20, LCY+23]. **dispersion-corrected** [GMO+20]. **dissipationless** [SG22]. **dissociation** [BHN23, BZW+20, CJVF+23, GRLH21, GOT+23, MM21, ZZLY22]. **dissociations** [JWZZ20]. **Distance** [LAAP21, RMWF20]. **distant** [DTAS21]. **distortions** [PZGH+20]. **distribution** [BRF21, CSS+21, Dau23, Gun21, MFC20a, RPT21b]. **distributions** [SDK+21]. **disubstituted** [MSADA21]. **disulfide** [AKK+21, PD22]. **disulfide/thiolate** [PD22]. **disulfides** [PD22, RK21]. **dithiafulvene** [ZKP22]. **dithiocarbamate** [MFJ+23]. **dithiophene** [XPZ20]. **diverse** [WLH+20]. **DMRG** [WFG+21]. **DMSO** [VOK+20]. **DNA** [LCH+22]. **Do** [AS22, LFMG20]. **docking** [BGM+23, CS23]. **dodecaboride** [YFX+22]. **dodecaborides** [PJ20a]. **dodecahedrane** [Ari21]. **Does** [KSPG23, LK20, RRSF22]. **domain** [GG20b, MJRS20]. **domination** [Kha23]. **domino** [HH23]. **donating** [XZ20]. **donor** [BSS21, CLL20, CZW21, DSNZ+20, LFRTRP+20, LYT+20, WZL23, XZ20]. **donor-** [LYT+20]. **donor-acceptor** [BSS21, LFRTRP+20]. **donor-bridge-acceptor** [CZW21]. **donors** [CLL20, KPMAB22, LL21, MJH+22, XPZ20, ZZ22]. **dopant** [LXWZ21, ZCL+22]. **doped** [AAJ+23, CWL+22, CZC+23, DYG21, ER22, GYC20, HFL23, KS21, KS23, LYPD23, MKKK22, MMP23, MCP+20, MAHRA+21, MIM21, MTA+22, NHH22, Pan20, PLZT22, RMS+23, RBJ21, RINHY20, SMP23b, SDL+22, SYD+23, THS20, VKS21, WWM+21, fXmTlS+23, XWS+22]. **doped-carbon** [EGLJQ+21]. **doping** [DYJ+22, GG20a, GRZ+21, KM21a, MHS21, MNWD20, RBJ23, RHS+21, RDMF21, WLY+20, YCPW20, ZZZ20b]. **dosimetry** [JAZ+20]. **dot** [BU20, BUKA21, Bah22, CWW+23, GKN+22, KB21, MIM21]. **dots** [CDD23, Mok21a, Ole21, RMM+22]. **double** [AAN+21, ARRB+21, FAB+23, FGW+22, GML+22, HMA+22, HMBPJ+20, KM23, KRB20, NM23, RCM+22, RKA+21, RSM+22, XgZX+22, ZFB+20, ZX21, ZCL+22, ZZL+20a, GSMT+20]. **double-hybrid** [HMA+22, HMBPJ+20]. **double-transition** [FGW+22]. **double-walled** [NM23]. **doubles** [BBG20, dSFdSdMdM20]. **doubly** [ATL+20, GOT+23, KKH21, WWKH22, Xav23]. **dppz** [DSNZ+20]. **dppz-based** [DSNZ+20]. **DR** [TCL+21]. **DR-2** [TCL+21]. **dragged** [PMdN21]. **dragging** [KAUB21]. **DRCNnT** [WZ20]. **dressed**

[Dau21, Dau23, HSV22]. **driven** [CDG+21, KRB20, TSN+21, WAM+20]. **driving** [CCZ20]. **drops** [ZL23]. **drug** [AGK23, LAAP21, MJA20, PSJ22]. **drugs** [CS23, Hav21, hHNRA23, KB23, KAA21, PB23, RNH23, TB22]. **dry** [HYC+21, RSD21]. **DSSCs** [HMA+22]. **dual** [NHNO20]. **during** [FCL22, SMS23]. **dye** [FZL+20, MSKA20, PIA21, PGPHAPM20, SIA20, YLL+20, SSS23]. **dye-sensitized** [FZL+20, MSKA20, PIA21, PGPHAPM20]. **dyes** [FZL+20, HMA+22, MSKA21, MKuAS+22, MRI20, PIA21, PGPHAPM20]. **Dynamic** [NHNO20, ATL+20, CMM21, SFB20]. **Dynamical** [HL20, sLsHtW+23, BPB+20]. **Dynamics** [PMdN21, CS23, CLS+22, DKK+20, Doh20, GRLH21, INV22b, JAZ+20, KPMAB22, LCH+22, LLC20, MZD+20, MW21, MKD21, Mok21c, dAOdASP+20, RSBK20, RKI20, RKG21, SASA21, TSN+21, TCL+21, TCX+22, WV20b, WAM+20, ZKP22, ZL23].

E-2 [SYT+21]. **E/Z** [HYHW22]. **E/Z-HFO-1234ze** [HYHW22]. **e26221** [Sur22]. **e26530** [Ano22a]. **earth** [LL21, MBKA21, MCP+20, NG20, RMS+23]. **easy** [GKK21, KSM+23]. **Eccentricity** [ZMS21, WYZZ20]. **Eccentricity-based** [ZMS21]. **Eckart** [NOO+23]. **edge** [MSOA23, RG20, RNA22, IAI20]. **edged** [DJC21]. **Editorial** [SSL22]. **education** [MNN+20, Shi20]. **Effect** [BPB+20, CP23, JBPV21, LHZG23, LQZ+21, NG20, SCAD+20, SFB20, SSS23, WCZ+20, BGK+22, BA21, CRKMC21, CLC+21, CLLC21, GN21b, HL20, JHH+22, KRS+21, KM23, KAUB21, LYT+20, LSS+21, LXWZ21, MSM+20, MWCJ23, MKM+20, MTA+22, MHD20, NIA21, PVR20, QDC+22, TPT20, UHK+22, WXLL21, YZD+21, YCSK20, ZZZ20b, DTAS21, EM21]. **effective** [DFB20, KV23, KAG+20, MZT20, VKK+21, ZAB+23]. **effectively** [LNC+23]. **Effects** [HLL+23, HDF+21, RHS+21, SGWW22, Wan21, YLL+20, YZL21a, BZW+20, DKK+20, FPdS21, HOVG20b, HLL20b, HLF23, JIFM22, KSP20, LCH+22, LZL+21, MKuAS+22, MZ23, MHS21, OAJ21, ONH+21, PCEAG23, QdOdMC+21, RSM+22, RKI20, SSIE20, SSEI21, STN20, SP20b, UIIP23, WZ20, WDS+20, WXLL21, WLLS21, WOE+22, XL22, YCPW20, ZMOE23, ZIA20, ZL21, ZCL+22, ZZZ+23, ZGCF20, tZNb+22]. **Efficiency** [TCSG+20, BCM23, KMH+20, SIA21]. **Efficient** [KLT21, NTND23, BA21, FZL+20, FAJOF20, KPMAB22, RS23, RKA+21, RINHY20, RF23, SNL+23, SYL+21, WP22]. **Eigen** [RNH23, Xav23]. **Eigen-value-based** [RNH23]. **eigensolver** [CJVF+23, GDR21, XgZX+22]. **eigensystem** [DS20]. **Einstein** [PMdN21]. **elastic** [BA22a, GGUU21, GUUG23, LWH+21, MSS22, MBM+21, SDK+21, SG20]. **elasticity** [SYD+23, WXHX22, YFX+22]. **Electric** [ZXS20, AMM21, CWY+20, EM21, FAX+23, Guh23, LNX+21, LCP21, MKM+20, Mok21a, NYX+21, RYC+20, TWT+21, VM20, WWZ+21, WP22, ZIA20, ZYZ+21a]. **electric-field** [FAX+23]. **electrical** [HFF22, Rac21]. **electride** [PC22, TSW+20]. **electrocatalyst** [CZJ+23]. **electrochemical** [KC23, MHS21, OKK+22, XQJ+21]. **electrochemotherapy** [ZYZ+21a].

electrode [dRNS21, SUG20, XWS+22]. **electrodynamic** [ZMOE23]. **electrodynamics** [SI20]. **Electron** [BA22a, DSNZ+20, MPBL23, SP20b, SA20, CCZ20, CPL+21, CLL20, CZW21, Cio22, FFBH21, Hua20, JVK22, JXM22, KZ21, KML23, LNE+20, LZ20, LL21, Lom21, LFMG20, MSS22, MSKA20, MSADA21, Nan23, PT21, PJ20b, QOM+20, Rad21, SDS19, SDS20, SCAD+20, SKG23, SBKT23, STT20, TWT+21, TAMU+23, TD22, UHK+22, UR23, XZ20, YÇDÖ21, ZIA20, ZS21, ZGCF20]. **electron-correlation** [ZIA20]. **electron-deficient** [LZ20, SBKT23]. **electron-donating** [XZ20]. **Electron-donor** [DSNZ+20]. **electron-hole** [CPL+21]. **electron-induced** [UHK+22]. **electron-transfer** [TWT+21]. **electron-withdrawing** [FFBH21, SCAD+20]. **electronegativity** [SMCNH22]. **Electronic** [AIR+23, CSY+21, DJC21, FK20, HLZZ23, MCP+20, RKA+21, RNFMC20, SBA21, Üng20, YZY+22, ZIA20, BPB+20, BBAA21, BA21, BWBR21, CDD23, CZGW22, CMGH+21, CP23, CLLC21, DDSB22, Dau21, DCY21, FPdS21, FH21, GYC20, GRZ+21, GGUU21, GUUG23, Gun21, HLL+23, HNO+21, HFL23, INV22b, JZX+20, KKH21, KLRS22, KM23, Kha23, KYL+20, KK21, KLK21, KM21b, KMG22, LLZC20, LCT+22, sLhZX+22, LWH+21, LDS+23, LDK23, LFMF23, MKKK22, MKuAS+22, MKM+20, MEBL22, MKD21, MK21, MIM21, MM21, MBM+21, MEWD20, MHG+23, NdVVT22, Nan23, NLA+21, ORL+20a, ONH+21, OMA21, Pan20, Pan22, PSN23, RPT21b, RSM+22, RMB+23, SAP22, SMP23a, SBG21, SCU21, dOSdASC+20, SG20, SMK+23, TMH21, TT21b, TVdVN21, TVdVN22, UBV+21, WXL+21, WYL22, WP20, WCM+23, WFG+21, Xav23, XFW+20, XBK+20, XWS+22, YLL+20, YCPW20, YCL+23, ZLH+20b, ZZZ20b, ZHFD+20]. **electronic** [tZNb+22]. **electronic/atomic** [UBV+21]. **electronic/atomic-scale** [UBV+21]. **electrons** [CFJ20, sLLqX+23, PJ20b, Sah21, SDK+21, TWT+21, UR23]. **electrophilic** [KZ21]. **electrophilicity** [JPSC20]. **electrostatic** [ABS20, Doh20, SSIE20, ZGCF20]. **element** [CMGH+21, WWLL21]. **elements** [BHN23, BA22a, DPC+20, KDY+22, MZT20, NG20, PL20, RPT21a, RPT21b, WWM+21, WWKH22, ZWL22]. **elephants** [Pev21]. **elimination** [AMM21, WAW+21]. **elucidated** [NHNO20]. **Elucidating** [MTA+22]. **elucidation** [HRTSS+20, SFPH22]. **Embedded** [RKI20, CZJ+23, DG21, GML+22, Hua20, ZQZ+23a]. **embedding** [Doh20, HOVG20b, Höf21, JMOW20, MJRS20, OAJ21, RVK23, SMJ20, WP20]. **embedding-based** [SMJ20]. **Emergences** [KOB20]. **emission** [DYJ+22, Jan22, SCZ21]. **emissive** [DSNZ+20]. **emitter** [SYL+21]. **emitting** [LK20, Üng23]. **empowering** [EPMC20, JHH+22]. **enable** [LLZ+20]. **enantioselectivity** [LLQ+21]. **encapsulated** [Ari21, ABDD22]. **encapsulating** [MI20]. **encapsulation** [BA21, CRKMC21, GMO+20]. **End** [KM21b, JHH+22]. **end-capped** [JHH+22]. **End-substituted** [KM21b]. **endohedral** [SBKT23, SBAT23]. **endohedrally** [RMS+23]. **energetic** [JXL+21, PLT+20, QLGZ23, SWXM23, WJL+21, XWJ+21, ZJW+21]. **energetics** [KML23, ÜB20]. **energies**

[AIB21, BHN23, BBG20, dSFdSdMdM20, FH21, FWY+22, GRFM20, HMBPJ+20, JXM22, LCP21, MFC20a, OB21b, PPCF+20, STN20, SGWW22, SPR22, TTTH20, TdV21, VCM+21]. **Energy** [Tak22b, YÇDÖ21, AAAAA23, AIB21, AA23, AB21, BFW+22, CZ21, CP23, CZW21, FWJ+23, HTNP21, HW21a, JHH+22, KRS+21, Kha23, KASAK23, KK23b, LCH+22, LCY+23, MC22, MZ21, MHD20, NF20, NR21, OR21, PT21, PZGH+20, RRD+22, Ram23, RKA+21, RK21, SFPH22, SSDF23, SPR21, SCU21, SKG21, Tak22a, TFF+22, VP20, WOE+22, WP22, XWLZ20, ZJW+21, ZZXT21, Zhu21, Tak22b, ZZJ+23]. **enforced** [MYS23]. **Engaging** [BHH20]. **engineering** [Cio22, JHH+22, PIA21]. **enhance** [GRZ+21, JHH+22]. **Enhanced** [AAB22, AJC+21, EGLJQ+21, FSR+22, RGLG23, SN21, WLY+20]. **Enhancement** [BSS21, PVR20, RMS+23, RBJ23, VdM22, YCL+22]. **enol** [KMK21, LZS20, SLdS20]. **ensemble** [LMA21, SF20a]. **ensembles** [CN21]. **entanglement** [AkAR+21]. **enthalpy** [WWL21]. **entropic** [KRB20]. **entropies** [hHNRA23, hHRN+23, IRA+20, INEB23, NZAH21, Ole20, SD20, TPCSD20, YHW+23]. **entropy** [AIN+20, EAPCD20, FMS+22, JSF+21, LSA+22, MSA22, QSZ23, RNA22, RR23, SJ20, SLPS20]. **envelope** [Dau21, GZCY22]. **environment** [BMF20, DFB20, STN20]. **environmental** [XHX+20, YZD+20]. **environments** [CLS+22, CBB21, MEBL22]. **enylidene** [BRB+21]. **enynes** [YYL21, ZZZW20]. **EOM** [TD22]. **EOM-CCSDfor** [TD22]. **EPc** [PC22]. **Epoxidation** [CSY+21, AAN+21, WLP+20]. **equalization** [SMCNH22]. **equation** [BBG20, CSS+21, Eti20, HRA+22, Izs21, KASAK23, LBP20, NACP21, OO21a, PM22, SS21, SGWW22]. **equation-of-motion** [BBG20, Eti20, SGWW22]. **equations** [BESG22, KLT21, SD20, TJA20]. **equilibrium** [BM21, EM21, KMK21, SP20a]. **equivalent** [LLZ+20]. **Erratum** [Ano22a, Ano23a, Bah22, Sur22]. **error** [DK21, Jan22, KA23, SM22]. **error-free** [SM22]. **errors** [LCP21]. **ester** [LMAA23]. **estimate** [GG20b]. **estimation** [HPAM23]. **Estrada** [LXZ21b]. **ethanol** [BTS+21, MFC20b]. **ethanol-to-butadiene** [BTS+21]. **ethers** [CMM+22, HZZZ22, TT21a]. **ethyl** [LMAA23, YLL+20]. **ethylene** [YZD+21]. **Eu** [LNC+23, AAJ+23, WZL23]. **Eu-doped** [AAJ+23]. **Europium** [DCY21]. **Europium-linked** [DCY21]. **EuRu** [KMG22]. **EuSi** [DCY21]. **Ev** [RNB22]. **Ev-degree** [RNB22]. **Evaluating** [BCM23]. **Evaluation** [VL21, BM21, KV23, ÖÇÖ21, Pev21, RDMF21, SSIE20, VKK+21]. **even** [WZ20]. **Evidence** [Hol21]. **evolution** [ASO+22, AKP22, DLZ+21, GYC20, LLX+23, LFMG20, ORL+20b, RSBK20, WYL22, fXmTlS+23]. **Exact** [CWY+20, GN20, KRS+21]. **examination** [ASHPHCB20, MGK23]. **Examining** [BMH21]. **example** [SBM22, dOSdASC+20]. **excellent** [WDS+20]. **exceptional** [Shi20]. **excess** [TWT+21]. **Exchange** [MMM20, AA23, Cin20, KRS+21, KA21, MMM16, NHNO20, ZPS+20]. **exchange-correlation** [AA23]. **excimer** [LK20]. **excitation** [BZW+20, CP23, FK20, HMBPJ+20, JBPV21, STN20, SGWW22].

excitations [BMF20, GDR21, XgZX+22]. **Excited** [VNK+23, BXWK22, DFB20, Eti20, FK20, HL20, Izs21, KGSD20, LBG20, Mka20, Nag20b, NZ20, NTND23, NYX+21, Rui22, SBG21, SKG21, TVdVN22, UHK+22, WY20, WWKH22]. **excited-state** [Eti20, Nag20b, NTND23]. **exciton** [BZW+20, CZ21, LYTS20]. **excitons** [KK23a]. **exhibiting** [ZQZ+23a]. **exhibition** [MOB21]. **Existence** [SMN+23]. **exohedrally** [RMS+23]. **expanded** [Cha21b]. **expansion** [AAAAA23, GM21, RSBK20, SSDF23, TLL23]. **expansions** [BCM23, SMJ20]. **expectation** [HTNP21, JIFM22, ZZJ+23, ZHJ+20]. **expected** [FYL21, LGW23]. **experiment** [ID21]. **Experimental** [LZS20, TCL+21, BY23, BBG20, DYJ+22, LZL+23, LSS+21, PPCF+20, RINHY20, RF23, WWZ+20, WAW+21, YHZ+22, ZAB+23]. **explain** [RRSF22]. **explanation** [LAKJ20]. **explicit** [OKK+22]. **explicitly** [BBTN23, JIFM22, Var21, WWF23]. **Exploiting** [HRA+22]. **Exploration** [CS23, BWLZ22, DYG21, Kan21, LZZ+20, MYS23, Röh21, ZWZB23]. **Exploring** [CZGW22, CJVF+23, DDSB22, EGLJQ+21, FSR+22, KS23, LCH+22, LYPD23, NHH22, SKG21, WZ20, ZGCF20, ZZ22, ZWL22]. **explosive** [HRTSS+20, MWC+21, WDS+20, ZGCF20]. **explosives** [WJL+21]. **exponential** [BKB+23, PGROM20, PMGR+21, XJ20]. **exponential-type** [PGROM20, PMGR+21, XJ20]. **Exponentially** [SPR21, SPR22]. **exponentials** [Lom21]. **expression** [Xav23]. **expressions** [YSZ23]. **extended** [KBR+20, LFRTRP+20]. **extent** [AD22]. **External** [MKM+20, ZXS20, ACM20, Bah22, EM21, KB21, PJ20b, TWT+21, WWZ+21, ZYZ+21a]. **external-potential-to-electron** [PJ20b]. **extinguishing** [CYL+23, HYC+21, LZL+23, TCX+22, WWZ+20, YHW+22, YHZ+22]. **extractants** [WZL23]. **extraction** [BA21]. **extrapolation** [QdOdMC+21, VP20, Var21]. **Extremal** [BDEM21, CSGR21, DL21, Ye20, Zhu21, BMR21, DTW21, ZZL20b]. **extremely** [LFX+21]. **extremum** [DAR+21]. **Eyringpy** [QDOC+21].

F [AMM21, CYL+23, GTC+23, PVR20, PLZT22, TWT+21, Yan20, ZWZB23, MBKA21, ÉC21, GZC21, MKD21, MNWD20, NZ20, SGWW22]. **f-orbital-dependent** [MBKA21]. **F12** [WWF23, KV23, VKK+21]. **F12c** [WWF23]. **Face** [DQS+21]. **faceted** [RF23]. **factors** [ZLG22]. **fail** [RRSF22]. **family** [WJL+21, XWLZ20, XWJ+21]. **Fan** [NR21]. **Fano** [CWW+23]. **fast** [BWR22, GKN+22, GKK21, KSM+23]. **Fatigue** [NYX+21]. **FCIQMC** [WFG+21]. **Fe** [MGK23, MGK23, MZ23, MIM21, MHG+23, SKR+21, SUG20, WWM+22, WCM+23, WFG+21]. **Feature** [HNO+21, CSY+21, JVK22, WWLL21]. **Feature-rich** [HNO+21]. **features** [MK21, Mok21a]. **featuring** [UR23]. **FeCrSe** [PKBZ20]. **FeCrTe** [PKBZ20]. **feedback** [GOR20]. **Feinberg** [NACP21, OO21b, OO21a]. **feldspar** [HYY20]. **FeNC** [GKPK21]. **fermionic** [BKB+23]. **fermions** [LMMA21]. **ferrate** [CSY+21]. **ferrimagnetism** [LHL+21]. **ferrites** [MHG+23].

ferrocene [WV20b]. **Ferrocenes** [Cha21a]. **ferroelectric** [MAHRA+21]. **ferromagnetic** [AMK+20, SG21]. **Ferromagnetism** [MNWD20]. **FeSi** [TMH21]. **Few** [TAMU+23]. **Field** [ZXS20, ACM20, AMM21, CRC21, CFJ20, CWY+20, Dau21, Dau23, EM21, FAX+23, GN21b, GOR20, Guh23, HK22, HP21, KKH21, LNX+21, sLsHtW+23, LCP21, MKM+20, Mok21a, NIA21, PPR21, SM22, TSN+21, TWT+21, WP22, ZIA20]. **field-dressed** [Dau21, Dau23]. **field-effect** [NIA21]. **Field-Phenyl** [ZXS20]. **fields** [Bah22, Bra21, KASAK23, KB21, NYX+21, RYC+20, VM20, WWZ+21, WOE+22, ZYZ+21a]. **fifth** [BHN23, Cio22]. **fifth-order** [Cio22]. **fifth-row** [BHN23]. **figure** [RMLPGHP20]. **filled** [KMG22]. **films** [DYJ+22]. **fine** [ZHJ+20]. **finite** [BCM23, VL21]. **finite-difference** [VL21]. **finite-temperature** [BCM23]. **fire** [CYL+23, HYC+21, LZL+23, TCX+22, WWZ+20, YHW+22, YHZ+22]. **fire-extinguishing** [CYL+23, LZL+23, TCX+22, WWZ+20, YHW+22, YHZ+22]. **First** [CZC+23, FMH+22, FAB+23, GSRG22, GGUU21, Kan21, KA21, KHH+21, LHL+21, LXWZ21, MBKA21, MHS21, OGSPP+22, Pan20, PM22, PS23b, RMeH+20, RED21, UV20, WXL+21, WWM+21, WCM+23, XCZ+21, YZL+21b, ZRR+21, AJC+21, AKKN20, BA22a, CSL+23, CDD23, CZGW22, CWL+22, DLZ+21, DAR+21, ER22, HLZZ23, HL20, JZX+20, JXM22, Kan22, KMG22, sLLqX+20, LHZG23, LYT+20, LWH+21, MSKA21, MIA23, MAHRA+21, MVF+23, MBM+21, MNWD20, NF20, NZ20, PL20, PS23a, RS21, RNFMC20, SFT+21b, SG21, SYD+23, WTC+23, XFW+20, ZYZ+21b, ZLH+20b, tZNb+22, KS21]. **first-hyperpolarizabilities** [LYT+20]. **First-order** [PM22]. **First-principle** [MHS21, RMeH+20, WXL+21, MBM+21, PS23a, XFW+20]. **First-principles** [CZC+23, FAB+23, GSRG22, Kan21, KHH+21, LHL+21, LXWZ21, MBKA21, OGSPP+22, Pan20, RED21, WWM+21, WCM+23, XCZ+21, YZL+21b, ZRR+21, AJC+21, AKKN20, CSL+23, CWL+22, DLZ+21, ER22, HLZZ23, JZX+20, Kan22, KMG22, LHZG23, LWH+21, MSKA21, MAHRA+21, PL20, RS21, SFT+21b, SYD+23, WTC+23, ZLH+20b, tZNb+22]. **first-row** [JXM22]. **Fisher** [NACP21, OO21b, AkAR+21, AIN+20, Nag22, OO21a]. **fit** [PJ20b]. **fitted** [Boz21]. **Fitting** [Pev21, KKK23, LSA+22]. **five** [JRA21, XPZ20]. **fixed** [ADZA21]. **Fizeau** [KAUB21]. **Fizeau-dragging** [KAUB21]. **Flat** [TT21a, SZMM22]. **flavonoid** [SIA20]. **flavonoid-based** [SIA20]. **flexible** [MBR21a]. **flexing** [LNX+21, YXKJ21]. **Flip** [XBK+20]. **fluctuation** [sLLqX+20]. **fluid** [TCL+21]. **fluorescence** [PCEAG23, SYL+21]. **fluorescent** [GA20, LXZ+21a, LYTS20, LZ23, TSHRS+20, ZLH20a]. **fluoride** [GHZ+23, LZL+21]. **fluorides** [SP20b]. **fluorine** [HNO+21]. **fluorine-** [HNO+21]. **fluorographene** [ID21]. **fluorouracil** [BSH+21]. **flutamide** [PSJ22]. **flux** [BM21, WOE+22]. **Fock** [BBTN23, JBPV21, RPT21a, RPT21b, Rui22]. **Fock-space**

[BBTN23, JBPV21]. **foldamers** [ZLG22]. **force** [Bra21, CCZ20, JD20, PPR21]. **forces** [RKK+22]. **forecasting** [AkAR+21]. **form** [BRHECY+22, LK20, MWBQ20]. **formalism** [AMM21, Eti20, MM22a]. **formamide** [SE20]. **Formamidinium** [ZCL+22, PAS+21]. **Formation** [SV21, WJF+21, FMM+23, LRG+20, LLW+21, MFE+23, SFB20, SBG21, WWL21, WZL+21]. **formed** [SMS23]. **formic** [SDL+22]. **forms** [KMK21]. **formulation** [BM21, UR23]. **Fourier** [SS21]. **FOX** [SWML23, ZZLY22]. **FOX-7** [SWML23, ZZLY22]. **fractal** [HAA+23]. **Fractional** [Mos21, SD20]. **fracture** [LYPD23]. **fragility** [JD20]. **fragment** [DFB20, NF20, PNC20]. **frame** [HTNP21]. **framework** [Boz21, GOT+23, HTNP21, HRTSS+20, HRA+22, KASAK23, SBA21]. **frameworks** [HW21a]. **free** [AKKN20, CPK22, dSFdSdMdM20, FMG23, HZC21, KM23, LT23, Nag20b, PIA21, PPCF+20, Ram23, SM22, TMX+22]. **free-standing** [HZC21]. **freedom** [Wan21]. **frequency** [WWF23]. **friendly** [GPP+21]. **Frontier** [SP20a]. **Frozen** [SMJ20, Höf21, OAJ21]. **Frozen-density** [SMJ20, Höf21]. **frustrated** [SSIE20]. **fuel** [SMS23]. **full** [BFW+22, LHL+21, SG21]. **full-dimensional** [BFW+22]. **full-Heusler** [LHL+21]. **full-Heuslers** [SG21]. **fullerene** [CRKMC21, DFK20, DYK22, GXL+22, GMO+20, GMRKMCMC21, PRC23, SBM22, VKS21, dPZFM+22]. **fullerene-ZnPc** [CRKMC21]. **fullerenes** [GMRKMCMC21]. **Fully** [MSS22]. **Function** [Tak22b, DS20, FWJ+23, KA23, NZ20, Sør21, SY21, Sur20, Sur22, Tak22a, WWM+21]. **Functional** [AMRS22, BVL22, TEEH23, Tak22b, AAJ+23, AAYA23, ABDD22, ARRB+21, BY23, BBAA21, BZP+20, BA21, BRB+21, BB20, BSH+21, CXZ+21, CPL+21, DRV20, DPC+20, DFK20, EGLJQ+21, EB22, FFBH21, FMM+23, GMO+20, GTV20, Jan22, JZL+21, KRS+21, KPMAB22, KVCS21, KYL+20, KAG+20, KS23, LT23, LLW+21, LK21, sLsHtW+23, LLX+23, LFRTRP+20, LCP21, LSS+21, LDS+23, MSKA20, MKKK22, MR21, MIM21, MOB21, MB23, MP20, MHG+23, Nag20b, Nag22, NHNO20, OKK+22, PM22, PJ20b, PD22, Pev21, PCEAG23, QdOdMC+21, QOM+20, RBJ23, RSD21, Röh21, SSEI21, SPF+22, SAP22, SK20, STN20, SK21, SF20a, Shi21, SSS23, SBJ20, SG20, STF21, Tak22a, TXW+20, THL+21, TSS+23, TCX+22, VGSS20, WZ20, XZ20, XQJ+21, XWS+22, YHW+23, YZD+21, ZZZ+20a, ZZLC20, ZXS21, ZHG+22, dPZFM+22]. **functionalized** [CSL+23, CSY+21, TEEH23, XZ20]. **functionals** [BXWK22, HMBPJ+20, Pev21, PRC23, SSDF23, ZYZ+22]. **functioning** [TPT20]. **functions** [CPK22, Gun21, LT23, NdVVT22, PS23a, TLL23, TFF+22, TVdVN21, TVdVN22]. **fundamental** [BFW+22]. **fundamentals** [CM21]. **fungal** [PB23]. **Further** [DYZ+23]. **fused** [PVR20, SWXM23, ZAB+23]. **Future** [KKRR21, JHH+22].

g [RINHY20]. **g-C** [RINHY20]. **Ga** [GSRG22, MBM+21, NG20, Yan20, LMM+22, sLLqX+20, SYD+23]. **Ga/In** [GSRG22]. **gallium** [NM23, SMP23a]. **GaN** [SMP23b]. **gap**

[LMM+22, OR21, RK21, SCU21, TAUM+23, WWLL21, WLY+20]. **Gas** [PLZT22, AN20, GOS20, LZL+21, MYS23, NHH22, PT21, RKI20, SASA21, Shi21, TTTH20, VdM22, XZGS23]. **gas-** [RKI20]. **gas-phase** [GOS20, LZL+21, SASA21, VdM22]. **gases** [dAOdASP+20, SCY+23, ZHW23]. **gate** [TPT20]. **Gaussian** [DGA23, KKK23, LT23, SSDF23, Sha20, TAMU+23]. **Gaussian-type** [Sha20]. **Gaussians** [JIFM22]. **Gd** [NG20]. **GDB17** [MJH+22]. **GDY** [HFF22]. **GDY-** [HFF22]. **Ge** [GUUG23, KLRS22, SYD+23, TSS+23]. **GeC** [TEEH23]. **General** [Ano22a, BT21, YSZ23, JLWH23, KH20, OB21b, TdV21]. **Generalized** [GN21a, GDR21, MZT20, ZMOE23, AGK23, GRFM20, HJIO21, IRA+20, KASAK23, WFG+21, WP22, XgZX+22, ZZJ+23, ZHJ+20]. **Generation** [KYL+20, GW21, LYW+20, NYX+22, SIM23, VSKG21, WAM+20]. **generative** [HBY20]. **genetic** [BSMI23, MSI22, RSBK20, TD22]. **Geometric** [RRS21, WYL22, BDEM21, GRLH21, RVK23]. **geometric-arithmetic** [BDEM21]. **geometrical** [CP23, ZZZ20b]. **geometries** [SP20a]. **geometry** [CN21]. **Germany** [KKRR21]. **GGA** [AAJ+23]. **GIAO** [GZC21]. **given** [CL22]. **glassy** [MZD+20]. **Global** [ZG21, DYG21, GHZ+23, KYL+20, KKK23, SMMP+23, TCL+21]. **globular** [Ye20]. **glutathione** [KI20]. **glycerol** [SBJ20]. **glycerol/hydrogen** [SBJ20]. **glycinamide** [ES21]. **glycine** [GOS20, NYX+22]. **glycolaldehyde** [ZWW+22]. **gmx2qmmm** [GPP+21]. **go** [GTV20]. **gold** [QOM+20]. **good** [Rac21]. **Gourava** [SZMM22]. **governing** [KLT21]. **gradient** [AMM21, MPBL23]. **gradients** [LCP21, RVK23]. **graduate** [CM21]. **grain** [PP23]. **graph** [AIAG21, AD22, CLW21, IAI20, LS21, PB23, RKI20]. **graph-theoretically** [RKI20]. **graphdiyne** [CZC+23]. **graphene** [ARBM21, CSTD22, DJC21, ID21, ISL+23, LZSA20, LK21, LXWZ21, MIA23, MI20, PSN23, PLZT22, QDC+22, RMM+22, RBJ21, RBJ23, SPF+22, SDL+22, WWM+22, XBL23, YZL21a]. **graphene-2D** [ISL+23]. **Graphitic** [LFX+21, YCPW20]. **graphs** [Ano22a, AD22, BDEM21, BT21, CL21, FYL21, Hao21, KB23, LCX+21, RRS21, RA20, WYZZ20]. **graphyne** [DRV20, HDF+21, HFL23, XCZ+21]. **graphynes** [HDF+21]. **grid** [LLC20]. **GridMol2.0** [ZMJ+20]. **Grignard** [KAG+20]. **Gromacs** [GPP+21]. **ground** [ACM20, KYL+20, LHL+21, Mka20, NZ20, Rui22, SPR21, SKG21, TVdVN21]. **ground-state** [KYL+20, LHL+21]. **Group** [STF21, Cha21b, HLF23, KDY+22, LLMQ20, PGPHAPM20, SLL+22, TT21b, YLL+20, ZLG22]. **group-11** [Cha21b]. **group-14** [KDY+22]. **Group-IV-based** [STF21]. **groups** [LFRTRP+20, XZ20]. **growth** [DYK22, DYG21, FCL22, LDK23, RMB+23, BRB+21]. **guess** [HK22]. **guided** [AAAAA23, DGA23]. **Gutman** [LGW23]. **GYs** [HDF+21].

H [ASO+22, Ari21, BFW+22, EB22, FK20, GNC20, GTC+23, JWZZ20, MOB21, PVR20, SNL+23, Shi21, SRS21, ÜB20, WCZ+20, WAW+21, YCSK20, Cha21a, CLS+22, DKK+20, Dau21, Dau23, KDY+22, LZL+21,

MSS20, dAOdASP+20, ÖÇÖ21, PLZT22, QDJY23, RS23, Roy20, SSIE20, SSIE21, SSK20, STF21, WY20, WXL+21, WZL+21, WSSD21, WOE+22, WHYL21, YZD+21, ISL+23, UHK+22]. **h-BN** [ISL+23]. **H-bond** [ÖÇÖ21]. **H-like** [CLS+22]. **H/** [UHK+22]. **H/D** [DKK+20]. **Half** [PKBZ20, Rui22, BB20, HBB+21, KLRS22, KDY+22, LMM+22, LHL+21, ONH+21, RCM+22, SG21, ZRR+21]. **half-Heusler** [PKBZ20, RCM+22, ZRR+21]. **half-metallic** [BB20, LMM+22, LHL+21, ONH+21, SG21]. **Half-metallicity** [PKBZ20]. **Half-Projected** [Rui22]. **half-sandwich** [KDY+22]. **halide** [AAM+20, BPB+20, KM23, PAS+21, ZZLC20]. **halides** [CFM+21, LL21, TMX+22]. **halogen** [KSP20, WXLL21]. **halogens** [KM23]. **Halon** [YHW+22]. **Hamiltonian** [AKP22, SM22]. **handedness** [ZLG22]. **hard** [KRA+23, MR21]. **hardness** [PJ20a]. **hardware** [RBSW21b]. **harmonic** [RNFMC20, SIM23]. **Hartree** [RPT21a, RPT21b, Rui22]. **harvesting** [FAB+23]. **HC** [PAS+21]. **HCl** [WY20, CMM+22, TFF+22, WY20]. **HCl-catalyzed** [CMM+22]. **HCNO** [MM20]. **He-like** [NdVVT22, TVdVN21, TVdVN22]. **heat** [END+23, YHW+23]. **heavier** [KDY+22, ZLT+20]. **heavy** [CFM+21]. **HeH** [MM21, Wan21]. **heights** [KV23]. **Heisenberg** [CSK21, JVK22]. **helical** [BCLM+22]. **helicenes** [GML+22]. **helicity** [XAM+22]. **helium** [CBB21, DG21, LBG20, MF21a, NZAH21, SPR21, TVdVN22]. **helium-like** [NZAH21]. **helix** [ZXS21]. **Hellmann** [Yal23]. **help** [Var23]. **Hermitian** [HRA+22, LMA21, SM22]. **hetero** [GML+22, JS21]. **heterocycle** [WJL+21]. **heterocycle-based** [WJL+21]. **heterocycles** [SSEI21]. **heterocyclic** [DDSB22, JRA21, LLZ+20, LLMQ20, PM20, SCAD+20, SWXM23, YLL+20, ZFB+20]. **heterodinuclear** [ZXS21]. **heterogeneous** [PGÁML21, WLP+20]. **heterogeneous-homogeneous** [WLP+20]. **heterojunction** [BZW+20, MI20, XHS+23, ZZZ+23]. **heterostructure** [ISL+23]. **heterostructures** [MIA23, OGSPP+22]. **Heusler** [BB20, GGUU21, GUUG23, HBB+21, KLRS22, LMM+22, LHL+21, MBM+21, PKBZ20, Rac21, RCM+22, ZRR+21]. **Heuslers** [SG20, SG21]. **HeX** [JWZZ20]. **hexaazaisowurtzitane** [ZGCF20]. **hexaborides** [MBKA21]. **hexacoordinate** [KRK+21]. **hexadienal** [SYT+21]. **hexafluoro** [LZL+23, WWZ+20]. **hexagonal** [BMR21, CPL+21, CDR20, DQS+21, FYL21, QSZ23, RMLPGHP20, SZMM22, ZFB+20]. **hexagons** [CL22, LC23]. **hexamer** [MFC20b]. **hexamolybdate** [AAYA23]. **hexamolybdate-julolidine** [AAYA23]. **hexanitro** [ZGCF20]. **hexyloxy** [LMAA23]. **hexylthiophene** [LMAA23]. **Hf** [GGUU21, PRC23, SCY+23, TFF+22, KHK+23, LLZC20]. **HFO** [HYHW22]. **HFP** [SK20]. **HfSe** [OGSPP+22]. **HfSSe** [OGSPP+22]. **HfTaZrNb** [JSF+21]. **HfTaZrTi** [JSF+21]. **Hg** [QOM+20, FAJOF20]. **Hierarchical** [TJA20]. **High** [LYT+20, XFW+20, XJLH21, BWR22, CZJ+23, GZWL22, HLL20a, HW21a, JSF+21, KMH+20, LFX+21, MZ21, PJ20a, Rac21, SIM23, SMP23b, SF20b,

SDL+23, ÜB20, XWLZ20, ZJW+21, ZLT+20, ZHG+22, ZZXT21]. **high-accuracy** [ÜB20]. **high-density** [XWLZ20]. **high-efficiency** [KMH+20]. **high-energy** [HW21a]. **high-energy-density** [MZ21, ZJW+21, ZZXT21]. **High-precision** [XJLH21]. **High-throughput** [XFW+20, BWR22]. **higher** [BXWK22]. **Highly** [GG20a, RS23, PAS+21, SC21]. **Hilbert** [SMN+23]. **Hirschfelder** [FWJ+23, TFF+22]. **history** [AB21, Rui22]. **HMDSO** [HCZ20]. **HNO** [WZL+21]. **HNSO** [MSS20]. **hole** [CPL+21, HLL20b, KSP20, LZ20, LL21, PSJ23, VM20, ZL21, ZZ22]. **hole-transporting** [LZ20]. **hollow** [LC23, SBKT23]. **holmium** [DYG21]. **holmium-doped** [DYG21]. **homogeneous** [PT21, WLP+20]. **homolytic** [KAG+20]. **homonuclear** [BA22b]. **honeycomb** [tZNb+22]. **Hooke** [TAUM+23, TAMU+23]. **Horodecki** [NACP21, OO21b, OO21a]. **HoSi** [DYG21]. **hosts** [CRKMC21]. **hot** [CLS+22, LYTS20]. **HRPA** [JS21]. **HS** [ZZZ+20a]. **Hückel** [WWKH22]. **Hulburt** [FWJ+23, TFF+22]. **Hulburt-Hirschfelder** [FWJ+23, TFF+22]. **Hulthén** [Yal23]. **human** [CS23]. **hyaluronic** [MA23]. **hybrid** [BGK+22, GKN+22, HMA+22, HMBPJ+20, QFA+23, WWF23, WZ21, AMRS22]. **hybridization** [XL22]. **hybrids** [AAYA23]. **hydrated** [GTAL23, SK20]. **hydrates** [ZLH+20b]. **hydration** [LK21]. **hydride** [CJVF+23, WJF+21]. **hydrides** [RMeH+20]. **hydroarylation** [LG21]. **hydroboration** [SSIE21]. **hydrocarbon** [ZL23]. **hydrocarbons** [Kha23, LCX+21, LPH22, LZZW23, RĐB+23, Var23, WYZZ20]. **hydrochalcogenation** [JRA21]. **hydrochlorination** [AKKN20]. **Hydrogen** [dAOdASP+20, SK20, TEEH23, BMF20, CSY+21, DLZ+21, EAPCD20, EAPCD21, FGMO20, HJL+23, JVK22, JXYL20, KHH+21, KLT21, LAKJ20, LWC+21, LLX+23, LYW+20, RS21, RMeH+20, RDMF21, SI20, SFB20, SRH20, SNL+23, SBJ20, WWM+22, XJLH21, fXmTlS+23, ZHG+22, STI20]. **hydrogen-like** [JVK22, XJLH21]. **Hydrogen/** [STI20]. **hydrogenated** [LFMF23]. **hydrogenation** [LSS+21]. **hydrogenic** [SLPS20, TPCSD20]. **hydrogenlike** [WKH20]. **hydrolase** [ÖÇÖ21]. **Hydrolysis** [MSS20, LZL+21, SASA21, ZZL+20a]. **Hydrolytic** [UAH+20, UIIP23]. **hydrophilic** [LCY+23]. **hydrophobicity** [JPSC20]. **hydrosilylation** [ZXS20]. **hydrothermal** [FCL22]. **hydroxide** [SKR+21]. **hydroxyacetone** [JD20]. **Hydroxyl** [XZGS23, SYT+21, ZTHW23]. **Hydroxyl-initiated** [XZGS23]. **hydroxylmethylfurfural** [LSS+21]. **hydroxymethylfurfural** [DYZ+23]. **hydroxyphenyl** [KMK21, PPR21]. **hydroxyquinoline** [SFPH22, UHK+22]. **Hylleraas** [BXWK22, SPR21, SPR22, ZGJ+20]. **Hylleraas-configuration** [SPR21, SPR22]. **hyperbolic** [IRA+20]. **hyperfine** [JAZ+20, ZHJ+20]. **hypergeometric** [SD23]. **hypergraphs** [LXZ21b, ZZL20b]. **hyperpolarizabilities** [LYT+20, MCP+20]. **hyperpolarizability** [BMF20]. **hypertrees** [Zhu21]. **hypothetical** [FGW+22]. **hypoxanthine** [ES21].

Identification [HCZ20, SI20]. **II** [LLMQ20, MFJ+23, MGK23, PPR21, Üng23, WFG+21, ZQZ+23a, ES21, KPTL23, LTC+23, MSOA23, PD22, SPR22, TVdVN22, ZPS+20]. **II.** [KV23]. **III** [DSNZ+20, LLW+21, LNC+23, MGK23, RKG21, WZL23, VSKG21, WLH+20]. **III.** [NdVVT22]. **IJQC** [Ano22a]. **Illuminating** [GA20]. **illustration** [SK20, UBV+21]. **Image** [Ano20a, Ano20l, Ano20p, Ano20q, Ano20r, Ano20s, Ano20t, Ano20u, Ano20v, Ano20b, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20m, Ano20n, Ano20o, Ano21b, Ano21q, Ano21r, Ano21s, Ano21t, Ano21c, Ano21d, Ano21e, Ano21f, Ano21g, Ano21h, Ano21i, Ano21j, Ano21k, Ano21l, Ano21m, Ano21n, Ano21o, Ano21p, HOVG20a, INV22a, MBR21b, MM22b, RBSW21a, SFT+21a, WV20a]. **imaging** [ZLH20a]. **imidazol** [KPTL23]. **imidazole** [KMK21, MSI22]. **imidazolium** [KSPG23]. **imidazolium-based** [KSPG23]. **impact** [MSS22]. **impenetrable** [YÇDÖ21]. **Implementation** [ZMJ+20, ABS20, Pon19, TPB+20, Yos20, ZS21]. **implication** [MM21]. **important** [HFF22, SMMP+23]. **imposed** [WY20]. **improve** [BXWK22, FWY+22, GZC21, MSKA20]. **Improved** [FFBH21, XJ20, CPK22, END+23, FWJ+23, GG20a, HJIO21, NR21, TFF+22, Yal23]. **improvement** [MSKA21]. **improves** [DYJ+22]. **Improving** [BKB+23, BBG20, dPZFM+22]. **impurity** [ZYZ+21b]. **In-silico** [MYS23]. **incidence** [Zhu21]. **incident** [SIA21]. **Including** [JWZZ20, SBG21]. **inclusion** [BRHECY+22, JIFM22, QOM+20]. **incorporated** [HNO+21]. **Incorporating** [ATL+20]. **Increase** [SUG20, KM21a]. **Increasing** [VdM22, OR21]. **indacenodithiophene** [FZL+20]. **indacenodithiophene-based** [FZL+20]. **indandione** [EM21]. **indenyl** [MZ23]. **index** [AIAG21, ADZA21, BDEM21, BMR21, DQS+21, FLZP23, GN21a, IAI20, IMJ21b, LPH22, LGW23, LC23, LXZ21b, WYZZ20, ZZL20b]. **indices** [AII21, Ali20, Ano22a, AGK23, BT21, CSGR21, DL21, DTW21, DAR+21, FYL21, Hav21, IMJ21a, INEB23, Jah20, KB23, KAA21, LSG21, LAAP21, LCX+21, LGW23, MB23, MA23, MAK+22, PS22, QSZ23, RNB22, RNH23, RA20, RMWF20, RĐB+23, TB22, Ye20]. **indirect** [OR21, WLY+20]. **indirect-to-direct** [WLY+20]. **indole** [WSSD21]. **Induced** [CPL+21, BUF+22, CBB21, KGSD20, MIA23, MNWD20, PM20, SYL+21, UHK+22, YCL+22]. **induction** [ZLG22]. **inequalities** [ZZJ+23]. **Influence** [BS20, CZW21, FAX+23, MIM21, MT21, PL20, WZL+21, BCM+22, BRHECY+22, CCZ20, CYJC20, CZ21, GYC20, ISL+23, KASAK23, PJ20a, ZPS+20]. **influenced** [AAM+20]. **Information** [Ano20w, Ano20x, Ano20y, Ano20z, Ano20-27, Ano20-28, Ano20-29, Ano20-30, 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, Ano21u, Ano21v, Ano21w, Ano21x, Ano21y, Ano21z, Ano21-27, Ano21-28, Ano21-29, Ano21-30, Ano21-31, Ano21-32, Ano21-33,

Ano21-34, Ano21-35, Ano21-36, Ano21-37, Ano21-38, Ano21-39, Ano21-40, Ano21-41, Ano21-42, Ano21-43, Ano21-44, Ano22b, Ano22c, Ano22d, Ano22e, Ano22f, Ano22g, Ano22h, Ano22i, Ano22j, Ano22k, Ano22l, Ano22m, Ano22n, Ano22o, Ano22p, Ano22q, Ano22r, Ano22s, Ano22t, Ano22u, Ano22v, Ano22w, Ano22x, Ano22y, Ano23b, Ano23c, Ano23d, Ano23e, Ano23f, Ano23g, Ano23h, Ano23i, Ano23j, Ano23k, Ano23l, Ano23m, Ano23n, Ano23o, Ano23p, Ano23q]. **Information** [Ano23r, Ano23s, Ano23t, Ano23u, Ano23v, Ano23w, Ano23x, Ano23y, LMA21, TAS21, AkAR+21, AIN+20, IRA+20, KRB20, MF21a, Nag20b, Nag22, NACP21, NZAH21, NOO+23, Ole21, OO21a, OO21b, PGÁML21, SLPS20, SD20, TPCSD20]. **infrared** [MFC20b, RYC+20, YXKJ21]. **infrared-active** [YXKJ21]. **inhibitor** [MFK22]. **inhibitors** [WV21]. **Inhibitory** [CLC+21]. **inhomogeneous** [DFB20]. **initial** [BWLZ22, DYK22, HK22, SWXM23]. **initiated** [XZGS23, YZD+20, YST+21, ZWZB23]. **initiation** [CLC+21]. **initio** [AAJ+23, BZW+21, CMGH+21, FGW+22, FWY+22, HZC21, JAZ+20, JSF+21, MZD+20, ORL+20b, PASS21, PSN23, RKI20, RKG21, SASA21, ZLT+20, ZKP22, ZWZB23, ZHS21]. **injection** [CPL+21, MSKA20]. **inlets** [CDR20]. **inner** [GTAL23]. **inner-core** [GTAL23]. **Innovation** [GG22]. **inorganic** [ZZLC20]. **inserted** [LSOEAE22]. **insertion** [SN21]. **insertion-enhanced** [SN21]. **Insight** [ARRB+21, BZP+20, BWBR21, HMN20, NIA21, SIA21, SSEI21, ZPS+20, BSS21, MSM+20, MWBQ20, Pan22, RG20, SMMP+23, SCU21, UIIP23, VKS21, WYL22, WLH+20, WHYL21, WZL23, ZYZ+21a, ZZ22]. **Insights** [LDK23, PGPHAPM20, QOM+20, ZHG+22, ZGCF20, ABDD22, FAJOF20, LZS20, LXZ+21a, MFE+23, MNWD20, RBJ21, RYC+20, SWML23, SYL+21, WSSD21, WFG+21, AIR+23, GMO+20]. **instantly** [BXWK22]. **Institute** [MNN+20]. **institution** [SF20b]. **insulation** [ZHD+23]. **insulator** [CRC21]. **Int** [GM21, Sur22]. **integral** [BM21, DKK+20]. **integrals** [Boz21, GM21, YSZ23]. **intensities** [TFF+22]. **Inter** [TWT+21, NM23]. **Inter-cage** [TWT+21]. **inter-wall** [NM23]. **Interaction** [BSH+21, ATL+20, AIB21, AB21, BVL22, CBB21, dSFdSdMdM20, GOT+23, ISL+23, KASAK23, MM22a, MYS23, MKD21, PSJ22, Rad21, RED21, SPR21, SPR22, UR23, ZXS20, ZGJ+20, dLRdLJ+20]. **interaction-induced** [CBB21]. **Interactions** [MWBQ20, Ale23, KA21, KDM+22, MC22, MF21b, MM21, MPBL23, NHNO20, OGT20, dAOdASP+20, RGS23, SK20, SC21, TLT+22, UP20, WWWC21, ZKP22]. **interactive** [BWR22]. **interatomic** [RKK+22]. **interconversion** [PD22]. **interconversions** [HYY20]. **Interface** [BZW+20, GPP+21, KAUB21, UBW+22]. **Interference** [KRA+23, BA22b]. **intermediate** [QOM+20, SKR+21]. **intermetallic** [BBAA21, sLLqX+20]. **intermolecular** [Kid21, TLT+22]. **internal** [Bra21, VM20]. **Interpretation** [AIB21]. **interruption** [ZHW23]. **intersections** [MM20, WAM+20]. **intersystem** [KWWZ20, LYTS20, SV21]. **intra** [ZZXT21]. **intra-annular** [ZZXT21]. **Intramolecular** [JD20, CCZ20, NTND23, QDJY23, SSIE20, UHK+22, YCSK20]. **Intriguing**

[HBY20]. **Intrinsic** [SDL+23]. **Introducing** [SMCNH22, Sur20, Sur22]. **introduction** [Nat22]. **invariant** [BFW+22, KKK23]. **invariants** [NS22, ZMS21]. **inverse** [LACP21, NG20, VN21]. **Inversion** [MMM20, BZW+21, Cin20, KH20, LLZ+20, MMM16, HKM+23]. **inversion-topomerization** [BZW+21]. **Inverted** [YCSK20]. **Inverting** [PJ20b]. **investigate** [THS20, ZRR+21]. **investigated** [KAA21, SRH20]. **Investigating** [CPK22, HOVG20b, KM23, KMG22]. **Investigation** [BB20, JXL+21, MKD21, MEWD20, SIM23, SG22, SG20, ZLH+20b, AN20, AJC+21, BTS+21, CLS+22, CBK+20, ER22, GNC20, GSRG22, HBB+21, HMBPJ+20, Kan22, Kid21, KML23, KPTL23, LC20, LYTS20, LCY+23, LLMQ20, LLQ+21, MFJ+23, MZ23, MOB21, OGSPP+22, Pan20, RMeH+20, Roy20, SCZ21, SKG23, SUSS23, SSS23, SBJ20, SYZF22, SLL+22, TT21b, TD22, UV20, WZL+21, YYL21, ZJW+21, dPZFM+22]. **investigations** [CZGW22, KWWZ20, KA21, LYT+20, LHL+21, LXWZ21, MSKA20, RCM+22, WWM+22, ZAB+23]. **involve** [LFMG20]. **involved** [CMM+22]. **iodine** [MF21b]. **ion** [BA21, EGLJQ+21, FMH+22, KSPG23, KRA+23, LXZ+21a, LFX+21, MHS21, dRNS21, P´23, SPR22, VdM22]. **ion-pair** [VdM22]. **ionic** [BSMB23, ÉC21, FK20, LNE+20, THL+21]. **ionization** [BBG20, MHD20, TD22]. **Ionized** [ÜB20]. **ions** [BVL22, CLS+22, HOVG20b, NZAH21, RED21]. **IOTC** [BCKN21]. **IOTC/CASSCF/CASPT2** [BCKN21]. **IQA** [LFMG20]. **IR** [CRGD+23, SN21, CZGW22, DSNZ+20]. **IRC** [QDOC+21]. **IRC-Analysis** [QDOC+21]. **IRMOF** [RDMF21]. **IRMOF-8** [RDMF21]. **iron** [KPTL23, MSOA23, VSKG21]. **irradiation** [LYW+20]. **iso** [NdVVT22, TVdVN21, TVdVN22]. **iso-electronic** [NdVVT22, TVdVN21, TVdVN22]. **Isobaric** [END+23]. **isocyanic** [ZLT+20]. **isolated** [PVR20]. **isomer** [MFC20a, TWT+21]. **Isomerism** [AS22]. **isomerization** [HKM+23, JD20]. **isomers** [BWLZ22, TLT+22, WYZZ20, dLRdLJ+20]. **isomorphic** [PASS21]. **isoprene** [SRS21, TXW+20]. **isospectral** [GN21a]. **isotope** [DKK+20, UHK+22]. **isotopomers** [NYX+22]. **isoxazolines** [MSADA21]. **Issue** [Ano20a, Ano20l, Ano20p, Ano20q, Ano20r, Ano20s, Ano20t, Ano20u, Ano20v, Ano20b, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20m, Ano20n, Ano20o, Ano20w, Ano20x, Ano20y, Ano20z, Ano20-27, Ano20-28, Ano20-29, Ano20-30, 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, Ano21b, Ano21q, Ano21r, Ano21s, Ano21t, Ano21c, Ano21d, Ano21e, Ano21f, Ano21g, Ano21h, Ano21i, Ano21j, Ano21k, Ano21l, Ano21m, Ano21n, Ano21o, Ano21p, Ano21u, Ano21v, Ano21w, Ano21x, Ano21y, Ano21z, Ano21-27, Ano21-28, Ano21-29, Ano21-30, Ano21-31, Ano21-32, Ano21-33, Ano21-34, Ano21-35, Ano21-36, Ano21-37, Ano21-38, Ano21-39, Ano21-40, Ano21-41]. **Issue** [Ano21-42, Ano21-43, Ano21-44, Ano22b, Ano22c, Ano22d, Ano22e, Ano22f, Ano22g, Ano22h, Ano22i, Ano22j, Ano22k, Ano22l, Ano22m, Ano22n,

Ano22o, Ano22p, Ano22q, Ano22r, Ano22s, Ano22t, Ano22u, Ano22v, Ano22w, Ano22x, Ano22y, Ano23b, Ano23c, Ano23d, Ano23e, Ano23f, Ano23g, Ano23h, Ano23i, Ano23j, Ano23k, Ano23l, Ano23m, Ano23n, Ano23o, Ano23p, Ano23q, Ano23r, Ano23s, Ano23t, Ano23u, Ano23v, Ano23w, Ano23x, Ano23y, HOVG20a, INV22a, KKRR21, MBR21b, MM22b, RBSW21a, SFT+21a, WV20a, Ano20-47]. **István** [CPK22, SSL22]. **iteration** [Yal23]. **Iterative** [HPAM23]. **IV** [ASHPHCB20, HLL20a, STF21, VSKG21]. **Ivan** [LUB23].

J [GM21, Sur22, BESG22]. **Jacobi** [SSD22]. **Jahn** [HL20, MM20]. **Jastrow** [NZ20]. **Jastrow-Backflow** [NZ20]. **joint** [RINHY20]. **jointed** [AJC+21]. **juglone** [dPZFM+22]. **julolidine** [AAYA23]. **junction** [NS22]. **JupyterLab** [HHG+21].

K-edge [MSOA23]. **Karplus** [BESG22]. **Karton** [KV23]. **Kekulé** [RRD+22]. **Kekulé-** [RRD+22]. **Keto** [KMK21, LZS20, SLdS20]. **Keto-enol** [KMK21, LZS20, SLdS20]. **ketones** [HZZZ22, LZ21]. **ketoxime** [YYL21]. **key** [SKR+21, ZLG22]. **kinase** [WV21]. **Kinetic** [BWLZ22, AAAAA23, MWC+21, SSDF23, Tak22a, VdM22, YST+21, ZTHW23, ZWZB23, Tak22b]. **kinetically** [KRK+21]. **Kinetics** [SRS21, KI20, SMS23, SXTZ23, YZD+20, ZZZ+20a, ZHS21]. **Kirchhoff** [FLZP23, Ye20]. **knowledge** [Nag20a]. **KOALA** [Höf21]. **KOBu** [VOK+20]. **KOH** [VOK+20]. **Kr** [dAOdASP+20]. **Kratzer** [AIN+20, GN21b].

L [MZ23, RR21, JAZ+20, MZ23]. **L-** [JAZ+20]. **L1** [KLT21]. **LAB** [CP23, Nag20a]. **lactamase** [KLT21]. **lactide** [MWCJ23]. **LaFe** [MTA+22]. **Lagrangian** [SY21]. **landscape** [RK21]. **landscapes** [Röh21]. **lanthanide** [Kov20, MWCJ23, SFPH22]. **lanthanum** [RKG21]. **LaO** [MEWD20]. **lapatinib** [HBY20]. **Laplacian** [LZSA20, LG22, LXZ21b]. **Laplacians** [FLZP23]. **Large** [LMM+22, RMLPGHP20, TSW+20]. **laser** [Dau21, GZCY22, HSV22]. **laser-dressed** [HSV22]. **lateral** [OGSPP+22]. **latest** [AGK23]. **lattice** [ACM20, FCL22, KS23, LHL+21, LXWZ21, ZX21]. **lattice-strain** [LXWZ21]. **lattices** [DQS+21]. **Laudatio** [LUB23]. **law** [LDK23]. **layer** [LMAA23, PSJ23]. **layered** [FMH+22, FGW+22, MEWD20]. **layers** [MKKA21]. **LC** [HMN20]. **LC-DFT** [HMN20]. **lead** [KM23, MNWD20, PAS+21, ZZLC20]. **lead-free** [KM23]. **lead-halide** [ZZLC20]. **leading** [MSADA21]. **learning** [AR22, BSMB23, BGM+23, FH21, FWY+22, KPMAB22, KSM+23, KK23b, LACP21, LLX+23, MJH+22, RP22, RKK+22, WWLL21, YZW+23, YHW+23, ZX21]. **Learn's** [KK23b]. **least** [PJ20b]. **least-squares** [PJ20b]. **length** [ZZ22]. **lepton** [BA22b]. **level** [LNE+20, LCY+23, ZLT+20, ZYZ+21a, ZYZ+21b]. **levels** [JS21]. **Lewis** [RKG21, SSIE20, WWWC21]. **Li** [Ari21, Yan21, ZXS21, AR22, ABDD22, FK20, FAB+23, HLL+23, MHS21, NdVVT22, OKK+22, PC22, RS21, RNRBFC21, SBA21, SPR22, TVdVN21, TVdVN22, ZYZ+22]. **Li-decorated**

[RS21]. **Li-like** [NdVVT22, TVdVN21, TVdVN22]. **Li-metal** [ZYZ+22]. **Li-polysulfide** [AR22]. **Li-S** [OKK+22]. **LiBH** [KHH+21]. **Libra** [DGA23, TJA20]. **life** [HYY20]. **lifetime** [LDS+23]. **ligand** [KKH21, KDM+22, MZ23, NHNO20, WHYL21]. **ligand-promoted** [WHYL21]. **ligands** [DSNZ+20, LNC+23, MWCJ23, SCAD+20, SGWW22, ZQZ+23a, ZPS+20]. **ligated** [DDSB22, Mok21a]. **Light** [KGSD20, BGK+22, CWW+23, FAB+23, Fin21, GKN+22, GRZ+21, LK20, LYW+20, Üng23, WAM+20, WZ21]. **light-driven** [WAM+20]. **light-emitting** [Üng23]. **Light-induced** [KGSD20]. **like** [AJC+21, ARBM21, Ano22a, BT21, CLS+22, CBK+20, DL21, JVK22, NdVVT22, NZAH21, dOSdASC+20, SSD22, TVdVN21, TVdVN22, WZ20, XJLH21, ZZJ+23, dPZFM+22]. **limit** [BT23, PMGR+21, Var21]. **limitations** [CJVF+23]. **limiting** [ZAB+23]. **Limonene** [FMG23]. **line** [HSV22, LS21, TFF+22]. **Linear** [AGK23, GXL+22, GML+22, OR21, ZGJ+20, AMM21, BSMI23, DS20, FLZP23, GZC21, HP21, LMMA21, LG22, MSI22, PM22, ZMJ+20]. **linear-scale** [ZMJ+20]. **linked** [DCY21]. **linking** [ZHD+23]. **liquids** [BSMB23, LNE+20, THL+21]. **Lithium** [ZHG+22, FMH+22, FAX+23, MZF21, MHS21, NdVVT22, dRNS21, OKK+22, RBJ21, Yan21]. **lithium-ion** [MHS21, dRNS21]. **lithium-sulfur** [MZF21]. **Ln** [Kov20]. **Local** [AIB21, SMMP+23, DK21, GTV20, Izs21, Roy20, SSDF23]. **local-density** [GTV20]. **Localization** [GN21b, KRB20]. **localized** [STI20, TWT+21]. **locked** [CP23]. **logic** [TPT20]. **Long** [XL22, EB22, KA21]. **Long-bonding** [XL22]. **long-range** [EB22, KA21]. **longevity** [Nag20a]. **loss** [YZW+23]. **Low** [PZGH+20, DB20, MM21, SCU21, TCL+21, TCSG+20, dLRdLJ+20]. **Low-energy** [PZGH+20]. **low-lying** [MM21, dLRdLJ+20]. **Löwdin** [Pon19, Yos20]. **Lower** [CDR20]. **lowest** [AMRS22, BXWK22, LYTS20, TVdVN22]. **luminescence** [DSNZ+20, SLL+22]. **luminescent** [SYL+21]. **LuZ** [MBM+21]. **lying** [MM21, dLRdLJ+20].

M [Ari21, HBB+21, HDF+21, KS21, LZZ+20, MZ23, OMA21, PZGH+20, PCKP20, QOM+20, Shi21, Tia21, Yan20, Ari21, HAA+23, LZZ+20, MZ23, MHG+23, OMA21, SLL+22, SYD+23, XL22]. **M-doped** [SYD+23]. **M-N** [KS21]. **M-polynomials** [HAA+23]. **Machine** [BSMB23, RKK+22, WWLL21, ZX21, AR22, BGM+23, FH21, FWY+22, KPMAB22, KSM+23, KK23b, LLX+23, MJH+22, RP22, YZW+23, YHW+23]. **macroscopic** [FWJ+23]. **made** [Mok21b]. **magic** [ELH20, WKH20]. **magnesium** [ZZZ20b]. **Magnetic** [LZS20, sLLqX+20, AJC+21, CSTD22, CPL+21, CLLC21, GGUU21, HOVG20b, HLZZ23, HNO+21, KA21, KASAK23, KC23, LBP20, MMP23, MBM+21, MT21, MHG+23, OAJ21, ONH+21, RG20, RMB+23, TMH21, VCM+21, WCM+23, WOE+22, Yan21, YZY+22, ZPS+20]. **Magnetically** [PM20]. **magnetism** [DYG21, GOR20, GYC20, PKBZ20, SDL+23].

Magneto [BU20, LTC+23, BBAA21, KMG22, SG20]. **magneto-electronic** [BBAA21, KMG22, SG20]. **Magneto-optical** [BU20]. **Magneto-structural** [LTC+23]. **Magnetoelectronic** [AMK+20, BB20]. **Maintaining** [SF20b]. **Majorana** [LMMA21]. **malonic** [SLdS20]. **malonitrile** [BRB+21]. **manager** [KS22]. **manipulation** [DRV20]. **Many** [UP20, RKI20, SMJ20, UR23, YÇDÖ21]. **Many-body** [UP20, RKI20, SMJ20]. **map** [PJ20b]. **Markovnikov** [LG21]. **material** [KDY+22, LFX+21, MJRS20, RSM+22, SCY+23, TD22, ZHG+22, ZHD+23]. **materials** [AKK+21, CRC21, EGLJQ+21, FSR+22, FAB+23, JHH+22, KMH+20, KM21a, LZ20, MMP23, MZF21, MHS21, RKA+21, RINHY20, SCZ21, SWXM23, SUG20, SC23, WWLL21, WJL+21, XZ20, ZJW+21, ZZXT21]. **mathematical** [Yos20]. **matrices** [BMH21, Eti20]. **Matrix** [BA22a, ATL+20, CL21, CMGH+21, Cio22, MWBQ20, SS21, TT21b, WWKH22]. **matter** [PMdN21]. **matter-wave** [PMdN21]. **MAX** [ARRB+21, FGW+22]. **maximum** [ADZA21]. **Maxwell** [BRF21]. **Mayer** [CPK22, SSL22]. **MB** [Tia21]. **McDonald** [BXWK22]. **mean** [CFJ20, sLsHtW+23]. **mean-field** [CFJ20, sLsHtW+23]. **means** [BVL22, GOT+23]. **measures** [FMS+22, LSA+22, MSA22, Ole21, RR23]. **Measuring** [AD22]. **Mechanical** [JSF+21, SMK+23, BCLM+22, CZGW22, CMGH+21, GUUG23, JZX+20, KLRS22, KHH+21, KHK+23, Kön21, KMG22, LZZ+20, MSCM23, ORL+20a, OMA21, PL20, PJ20a, Pan22, PKBZ20, PP21, TFF+22, WCM+23, XFW+20, YCL+22, ZRR+21, ZLH+20b]. **Mechanically** [PAS+21]. **mechanics** [BRF21, LACP21, NF20, RKK+22, ZMJ+20, GPP+21]. **mechanics/Gromacs** [GPP+21]. **Mechanism** [LZ21, MWCJ23, YZD+20, ZZZ+20a, ZZL+20a, ZHS21, BZP+20, CSY+21, CMM+22, DYZ+23, ES21, GYC20, HH23, HRTSS+20, HYC+21, JRA21, JXYL20, KI20, LWW20, LZL+21, LLQ+21, SSEI21, SWML23, SE20, SRS21, SYL+21, SYT+21, SXTZ23, TXW+20, TSS+23, TCX+22, TSHRS+20, TMX+22, WLP+20, WWM+22, WSSD21, fXmTlS+23, YZL+21b, YHW+22, YHZ+22, ZHD+23, ZWW+22, ZWZB23, ZL23]. **Mechanisms** [SBG21, LLLL20, LFMG20, VOK+20, WCZ+20]. **Mechanistic** [BTS+21, WLH+20, WHYL21, ZTHW23, AAN+21, HW21b, LG21, YST+21]. **media** [KAUB21, Üng20]. **mediated** [ER22, PD22, Ram23]. **MEH** [LMAA23]. **MEH-PPV** [LMAA23]. **melem** [AII21, MAK+22]. **melting** [PP21]. **membered** [JRA21, ZZL+20a]. **memoriam** [SSL22]. **MERCURY** [Shi20, LXZ+21a, QOM+20, Ano20-47, MNN+20]. **merit** [RMLPGHP20]. **mesogenic** [RKG21]. **mesoionic** [dSFdSdMdM20]. **metabolism** [HBY20]. **metabolite** [HBY20]. **Metadynamics** [ZLG22]. **metal** [AKKN20, Ari21, ARRB+21, BTS+21, CYJC20, CZJ+23, DTAS21, FK20, GTAL23, HLZZ23, HRTSS+20, JZX+20, JXM22, Kan22, KM21a, sLLqX+23, LL21, MFJ+23, NG20, OAJ21, PIA21, Pan20, PC22, PS23b, SCAD+20, SSDF23, SRH20, SLL+22, SDL+23, TMX+22, UBW+22, VN21, WWM+22, WWM+21, fXmTlS+23, XQJ+21, YZY+22, ZYZ+22]. **metal-anthracene**

[YZY+22]. **metal-doped** [Pan20]. **metal-free** [AKKN20, PIA21, TMX+22]. **metal-nitrogen** [PC22]. **metal-organic** [HRTSS+20]. **metal-salen** [CYJC20]. **metallated** [Üng20]. **metallic** [BB20, CYJC20, CWW+23, LMM+22, LHL+21, MBR21a, Mok21b, ONH+21, SG21]. **metallicity** [PKBZ20]. **metallo** [KLT21, PC22]. **metallo-** [KLT21]. **metallo-organic** [PC22]. **metalloporphyrin** [GMO+20]. **metalloporphyrin-based** [GMO+20]. **metalloproteinase** [MWBQ20]. **metalloproteinase-7** [MWBQ20]. **metals** [DRV20, FGW+22, GRZ+21, KM21a, MKKK22, MMP23, RMS+23, RHS+21, SAP22, SMP23b]. **Metastable** [FMM+23]. **methacrylate** [DFK20]. **Methane** [DB20, RSD21, RDMF21, XCZ+21]. **methanol** [CLL23]. **Method** [MMM20, ATL+20, Ano22a, BFW+22, BBTN23, BT21, BBG20, Cin20, FWY+22, GM21, KA23, KH20, LDS+23, LLC20, MMM16, NF20, NLA+21, Pon19, PS23b, Rad21, Rui22, STI20, SY21, SYL+21, TCSG+20, Yal23, ZZJ+23, ZHJ+20]. **methodology** [DGA23]. **Methods** [ZG21, Boz21, CDD23, CLS+22, Eti20, FH21, GZC21, GTC+23, HP21, LSA+22, PPCF+20, Pev21, Röh21, SRH20, SS21, WWL21, WP20, WWF23, ZMJ+20]. **methotrexate** [MA23]. **methoxy** [LMAA23]. **methoxyethyl** [YST+21]. **methyl** [CLL20, DFK20, HMA+22, LMAA23, MSM+20, SRS21]. **methylidyne** [ASO+22]. **metronidazole** [MJA20]. **MFe** [MHG+23]. **Mg** [Ari21, PCKP20, Tia21, AAB22, HYC+21, KAG+20, PLZT22, RMS+23, SNL+23, SYD+23, WWM+21]. **Mg-doped** [PLZT22]. **MgB** [LWH+21]. **MgTi** [Kan21]. **MgV** [Kan21]. **MH** [PCKP20]. **microhydration** [MHD20]. **microscopic** [ZL23]. **Microsolvation** [CFM+21, VCM+21]. **microstructural** [YZL21a]. **microwave** [FCL22]. **microwave-hydrothermal** [FCL22]. **migration** [KVCS21, RBJ21]. **mimic** [KI20]. **mimics** [ÖÇÖ21]. **minima** [DYG21, SDK+21]. **minimization** [KRB20, PJ20b]. **Minimum** [RPT21a, RPT21b, SYD+23]. **mining** [MJH+22]. **misfolding** [Hol21]. **mitigator** [UBV+21]. **Mixed** [sLsHtW+23]. **mixtures** [BSMB23]. **MM** [CN21, Ram23, SYL+21]. **Mn** [CZC+23, KC23, LHL+21, MBM+21, ONH+21, SG20, WWZ+21]. **Mn-based** [SG20]. **Mn-corrolazine** [WWZ+21]. **Mn-modified** [CZC+23]. **MNg** [Yan20]. **MnGe** [TT21b]. **MnO** [MHS21]. **MnX** [GGUU21]. **Mo** [OMA21, PP21, PPCF+20, PP21]. **mobility** [RSM+22, ZZ22]. **Mobius** [NOO+23, QSZ23, FLZP23]. **model** [AkAR+21, ABS20, BCM23, END+23, KGSD20, KKK23, NSM22, OKK+22, RVK23, SMCNH22, TSN+21, TAS21, TFF+22, Xav23, BVL22]. **Modeling** [KMK21, LMAA23, RGS23, Ale23, BSMI23, BBTN23, Doh20, Hav21, KI20, LL20, MJH+22, MEBL22, ORL+20a, SBKT23, Sta21, TPB+20]. **models** [AGK23, FK20, Fin21, KK23b, MSI22, PB23, RF23, VL21, VOK+20]. **moderate** [DB20]. **modes** [WZ21, YXKJ21]. **modification** [HBY20, MSKA20, ZAB+23]. **Modified** [BBTN23, CZC+23, HFL23, LCY+23, NOO+23, XCZ+21]. **Modulating** [SMP23b]. **Modulation** [LZ20, BSS21]. **moiety** [FFBH21, ZAB+23]. **molar**

[END+23, YHW+23]. **Molecular** [DTW21, FZL+20, FAJOF20, HTNP21, HLL20a, JXL+21, LCY+23, PIA21, RPAA22, RP22, SIA20, SSIE20, WV20b, XWLZ20, ZZXT21, ZZZ+23, Ano22a, BBTN23, BMH21, Boz21, BT21, CS23, CZ21, DKK+20, FMS+22, GOT+23, GOR20, GDR21, Gun21, GZCY22, GM21, HZZZ22, IMJ21b, ISL+23, JAZ+20, JJJM21, JLWH23, KZ21, KB23, KPMAB22, KKK23, LCH+22, MZD+20, MW21, MNN+20, MWC+21, MSADA21, MB23, MA23, NF20, RA20, RKI20, RKG21, RC20, SMN+23, SP20a, Shi20, SA20, TCL+21, TCX+22, TPT20, WWL21, WAM+20, WY20, WP22, YZY+22, YSZ23, ZMJ+20, ZYZ+21a, ZKP22, ZL23, MNN+20]. **Molecular-scale** [SIA20]. **molecule** [BCKN21, FWJ+23, GRLH21, KPMAB22, LC20, ÖÇÖ21, TSS+23, Var23]. **molecules** [AGK23, AMM21, BUF+22, BCM+22, BA22b, CWL+22, CBB21, CJVF+23, Doh20, GOS20, GKN+22, HSV22, HTNP21, HJIO21, ID21, JS21, KJA+21, KASAK23, LZ20, Mok21b, MAMB+22, NHNO20, NR21, PNC20, Rad21, RED21, SSIE21, Sta21, TFF+22, TTTH20, WAM+20, WOE+22, XJ20, Yan21]. **Molint** [Boz21]. **Møller** [HLL20a]. **molybdate** [HOVG20b]. **molybdenum** [AKK+21, RK21]. **Moment** [RSBK20, AJC+21, CZ21, HTNP21]. **moments** [AKP22, BCM+22]. **momentum** [Dau23]. **MoN** [SMK+23]. **monkeypox** [KB23]. **monobasic** [HZZZ22]. **monoborides** [XQJ+21]. **monocation** [WAW+21]. **monoclinic** [Pan22, ZX21]. **monocyclic** [MFE+23]. **monofluorinated** [SYZF22]. **monohydroxycinnamic** [BVT20]. **monoketone** [LWR21]. **monolayer** [CLLC21, HZC21, MKKK22, MNWD20, NHH22, RS21, RS23, SIM23, SPF+22, UP20, tZNb+22]. **monolayers** [XHX+20]. **Monomer** [XHS+23]. **mononitride** [sLhZX+22]. **Monosubstituted** [Cha21a]. **monoxide** [THS20]. **Monte** [SRH20, HZC21, KA23, NZ20, SS21]. **Monte-Carlo** [SS21]. **MoO** [HOVG20b, WLP+20]. **MoPro** [Shi21]. **MoPro-H** [Shi21]. **morphology** [XHS+23]. **Morse** [BU20, PMGR+21, SS21]. **MoS** [MIA23, UP20]. **Mössbauer** [GKPK21, KPTL23]. **most** [SBM22]. **Mostar** [AIAG21, AII21, DL21, IAI20, MAK+22]. **motion** [BBG20, Dau21, Eti20, FGMO20, Izs21, KK23a, RRSF22, SGWW22, TJA20]. **motor** [WAM+20]. **movement** [BS20]. **Moving** [LLC20]. **MP2** [QdOdMC+21]. **MRhSb** [HBB+21]. **MSbO** [PZGH+20]. **multi** [ABDD22, JBPV21, MKD21, Nan23, SZMM22, ZS21, dLRdLJ+20]. **multi-configuration** [ZS21]. **multi-Diels** [ABDD22]. **multi-dimensional** [SZMM22]. **multi-electron** [Nan23]. **multi-reference** [JBPV21, dLRdLJ+20]. **multicenter** [YSZ23]. **Multidimensional** [LLC20, MJH+22, TPCSD20]. **multielectron** [GM21]. **multifunctionalized** [MZ21]. **Multilevel** [HK22, Kön21]. **multinitro** [XWLZ20]. **multinitro-triazole** [XWLZ20]. **Multinuclear** [ZQZ+23a]. **multiparameter** [PMGR+21, XJ20]. **multiphoton** [JWZZ20]. **Multiple** [LYT+20, BSMI23, KSM+23, MZ23, MSI22, SD20]. **Multipole** [HJL+23]. **multireference** [dSFdSdMdM20, GDR21, JJJM21]. **Multiscale**

[Doh20, CN21, ZLH20a]. **multivalent** [KM21a]. **mutations** [LCH+22]. **MXene** [LLZC20, YCL+23]. **MXenes** [LLX+23, LZZ+20].

N [APR20, EB22, Kov20, KS21, NG20, RINHY20, WWWC21, YCPW20, dPZFM+22, Yan21, CZC+23, CPL+21, ÉC21, GML+22, JRA21, LFRTRP+20, LLMQ20, LXWZ21, MSM+20, MSS22, MNWD20, NHNO20, NZ20, RG20, SSIE20, SSEI21, SDL+22, SBG21, TCX+22, WOE+22, WZL23, XHX+20, XQJ+21, ZHG+22, ZWZB23]. **N-containing** [SSEI21]. **N-donor** [WZL23]. **N-dopant** [LXWZ21]. **N-doped** [CZC+23, SDL+22]. **N-embedded** [GML+22]. **N-heterocyclic** [JRA21]. **Na-ion** [LFX+21]. **Nakatsuji** [Sør21]. **nano** [KAUB21, dPZFM+22]. **nano-cage** [dPZFM+22]. **nano-composites** [KAUB21]. **nanocavity** [CWW+23]. **nanoclusters** [DYG21, ER22, FPdS21, SNL+23]. **nanocomposites** [CSTD22, UBW+22]. **nanocone** [SUSS23]. **nanocones** [Ali20, Jah20, TEEH23, ZMS21]. **nanocrystal** [FCL22]. **nanoflakes** [CSTD22]. **nanohoop** [ZQZ+23a]. **nanohybrids** [Mok21b]. **nanomaterials** [MZ21]. **nanometer** [ISL+23]. **nanoparticle** [RF23]. **nanoparticles** [CWW+23, LCY+23]. **nanoparticles-quantum** [CWW+23]. **nanoplastics** [Hol21]. **nanoring** [Mok21b]. **nanosheet** [MMP23, RR23]. **nanosheets** [DJC21, PSN23]. **nanosize** [DCY21]. **nanostructures** [AII21, IAI20, KOB20, MAK+22, ZZLC20]. **nanotori** [Ali20, Jah20]. **nanotube** [KS21, MJA20]. **nanotube-based** [KS21]. **nanotubes** [AA20, DQS+21, IMJ21a, IMJ21b, KS23, MCP+20, NS22, NM23, Roy20, SMP23a, SMP23b, SZMM22, THS20]. **naphthalimide** [PCEAG23]. **NaTm** [KC23]. **natural** [LFRTRP+20, Roy20, SIA20, SMCNH22, SK21]. **Nature** [GMO+20, PCKP20, QOM+20, RR21, Ari21, BPB+20, CRKMC21, MT21, NHNO20, RNRBFC21]. **Nb** [HBB+21, TMH21]. **NbCoSn** [ZRR+21]. **NbFeSb** [ZRR+21]. **NbS** [dRNS21]. **NbSi** [LHL+21]. **NCO** [KRS+21]. **Nd** [SMK+23]. **NdCo** [BBAA21]. **NdRu** [KMG22]. **near** [BT23, BM21, KRA+23, PZGH+20]. **near-equilibrium** [BM21]. **nearsightedness** [HRA+22]. **necessary** [Sør21]. **negative** [KRA+23, MOB21]. **neighboring** [BCM+22]. **network** [AkAR+21, BSMI23, BFW+22, HW21a, JLWH23, MSI22, WWL21]. **networks** [BKB+23, FLZP23, LPH22, ÖÇÖ21]. **Neumann** [Ole20, Ole21]. **neural** [AkAR+21, BSMI23, BFW+22, BKB+23, JLWH23, MSI22, WWL21]. **neurotransmitter** [CRGD+23]. **neutral** [AN20, ABDD22, FK20, FAX+23, KDY+22, KMK21, MZXL21, MFC20a]. **newly** [SG20]. **Next** [WAM+20, NYX+22]. **Next-generation** [WAM+20, NYX+22]. **NFAT5** [LCH+22]. **NFAT5-DNA** [LCH+22]. **Ng** [dAOdASP+20, XL22, Yan20]. **NH** [PAS+21, PLT+20, RR21, MSS20, WZL+21, fXmTlS+23]. **NHC** [LZ21]. **NHC-catalyzed** [LZ21]. **Ni** [EB22, KYL+20, KC23, DB20, EB22, MHG+23, RSD21, UBV+21, fXmTlS+23]. **Ni-W** [UBV+21]. **NiB** [LCT+22]. **nickel** [LG21, RMB+23, TEEH23]. **nickel-catalyzed** [LG21]. **nickel-phosphorus**

[RMB+23]. **NiI** [MKM+20]. **Niko** [Ano22a]. **niobium** [KS23]. **nitrate** [SK20]. **nitric** [LZ23]. **nitride** [CPL+21, MMP23, MCP+20, SMP23a]. **nitro** [JXL+21, QLGZ23]. **nitro-1-** [QLGZ23]. **nitroalkenes** [KZ21]. **nitroaromatics** [ZKP22]. **nitrogen** [DYJ+22, HNO+21, KS23, PC22, SBG21, THS20, WXLL21, ZJW+21, ZZXT21]. **nitrogen-incorporated** [HNO+21]. **nitrogen-rich** [ZJW+21]. **nitroso** [HBY20, YCSK20]. **nitrosyl** [RR21]. **nitrotriazoles** [XWJ+21]. **Nix** [KS22]. **NiZ** [GUUG23]. **NMR** [CRKMC21, CRGD+23, GZC21, GMRKMCMC21, HMN20, SSK20, SK21]. **NMR-shielding** [CRKMC21]. **NO** [RR21, YST+21, CWL+22, Kid21, MZ21, NHH22, SXTZ23, WZL+21, WOE+22, ZZLY22]. **noble** [AN20, HLZZ23, MYS23, dAOdASP+20, TTTH20]. **noble-gas-containing** [TTTH20]. **Non** [CMM21, BA22a, BCLM+22, GXL+22, LMA21, MC22, MM21, NG20, RKA+21, SSDF23, XAM+22, SPR22]. **Non-adiabatic** [CMM21, MM21]. **non-aqueous** [BCLM+22]. **non-central** [BA22a]. **non-covalent** [MC22]. **non-fullerene** [GXL+22]. **non-Hermitian** [LMA21]. **non-local** [SSDF23]. **non-metal** [NG20]. **Non-relativistic** [SPR22]. **non-scalar** [XAM+22]. **non-toxic** [RKA+21]. **nonadiabatic** [MKD21]. **nonadjacently** [ZMS21]. **noncentral** [GN20]. **Noncovalent** [ZKP22, Ale23, MYS23, OGT20, TCSG+20]. **nondoped** [SYL+21]. **nonelectrostatic** [VL21]. **Nonempirical** [HMBPJ+20]. **nonideal** [DG21]. **Nonlinear** [BMF20, AAYA23, BRB+21, GXL+22, GML+22, HDF+21, HFF22, HLF23, HFL23, LYT+20, MVF+23, RMS+23, SFB20, TSW+20, ZXS21, ZQZ+23a, ZAB+23]. **nonlocal** [Hua20]. **nonmetal** [CWL+22]. **nonmetallic** [LK21]. **nonorientable** [QSZ23]. **nonpolar** [LLZ+20]. **nonrelativistic** [SPR21]. **NOO** [YCSK20]. **Normal** [Bra21]. **normalized** [LZSA20, LG22]. **norms** [SSD22, SD23]. **novel** [AAYA23, FZL+20, HBB+21, Hav21, TSW+20, WJL+21, ZLH20a, ZLH+20b]. **Nuclear** [DKK+20, UHK+22, FGMO20, OAJ21, RKI20, RRSF22, SSIE20, VCM+21, ZQZ+23b]. **nucleation** [JLWH23]. **nuclei** [OAJ21]. **nucleobase** [UAH+20]. **nucleon** [GRFM20]. **nucleophiles** [LWC+21]. **number** [CL22, CDR20, ELH20, HDF+21, sLLqX+23]. **numbers** [WZL23]. **Numerical** [SS21].

O [FK20, GNC20, JXYL20, JZL+21, Kan21, KC23, LZL+21, MKD21, MTA+22, MHG+23, SKR+21, SUG20, ÜB20, WCZ+20, YST+21, YZL+21b, ZZZ+20a, ZYZ+21b, ÉC21, LZL+21, NZ20, WXL+21, WZL+21, ZYZ+21b]. **O-rich** [ZYZ+21b]. **O3** [KC23]. **O3-phase** [KC23]. **obtained** [ZYZ+21b]. **Obtaining** [YHW+23]. **occupation** [sLLqX+23]. **occupied** [ATL+20, GOT+23]. **octafluoro** [GB21, YHW+22]. **Octafluoro-2-butene** [YHW+22]. **octafluoro-spirobi** [GB21]. **octagonal** [FLZP23]. **octagonal-quadrilateral** [FLZP23]. **octane** [WYZZ20]. **odd** [WZ20]. **off** [Cio22]. **off-diagonal** [Cio22]. **OH** [HYC+21, YST+21, MOB21, YZD+20, ZWZB23]. **OH-bonded** [MOB21]. **OH-initiated** [YZD+20]. **oil** [ZL23]. **oils** [AAN+21]. **OLED** [SCZ21].

OLEDs [LYTS20]. **oligoamide** [ZLG22]. **oligomer** [WZ20]. **oligomer-like** [WZ20]. **oligomeric** [ZQZ+23a]. **oligomers** [MWBQ20, OR21]. **oligophenylenes** [INV22b]. **oligothiophene** [ZZ22]. **OM** [HDF+21]. **omicron** [TB22]. **One** [LBG20, Cio22, Eti20, JXL+21, LZZW23, LFMG20, Ole20, PMGR+21, SKG23, UR23, WCZ+20, YZY+22]. **one-** [LZZW23]. **one-body** [Eti20]. **one-dimensional** [Ole20, PMGR+21, YZY+22]. **one-electron** [Cio22, UR23]. **one-step** [LFMG20, WCZ+20]. **ONIOM** [THS20]. **Open** [YZW+23, MJRS20, SF20a, HHG+21]. **Open-circuit** [YZW+23]. **opening** [CYJC20, dSFdSdMdM20, MWCJ23, MAMB+22]. **operations** [AIAG21, AD22, IAI20]. **operator** [Yos20]. **opposite** [WXLL21]. **Optical** [BUKA21, INV22b, KB21, Mok21a, QFA+23, AAYA23, AIR+23, BU20, BRB+21, CDD23, CZGW22, GXL+22, GML+22, GGUU21, GUUG23, HLL+23, HNO+21, HDF+21, HFF22, HLF23, HFL23, KM23, LLZC20, LYT+20, MKuAS+22, MAHRA+21, MRI20, MVF+23, MIM21, MTA+22, MSCM23, MHG+23, Pan20, RMS+23, RSM+22, SFB20, TSW+20, Üng20, WV21, ZAB+23, ZZLC20, ZQZ+23a, ZLH+20b, tZNb+22, Bah22]. **optical-phores** [LYT+20]. **optics** [ZXS21]. **Optimal** [VP20, WWLL21]. **optimally** [TSN+21]. **optimisation** [TSN+21]. **Optimization** [GSMT+20, AJC+21, SS21, SUG20, ZG21]. **optimized** [GDR21]. **Opto** [ZHFD+20]. **Opto-electronic** [ZHFD+20]. **optoelectronic** [AAJ+23, AAB22, AAM+20, AIR+23, HBB+21, KHH+21, KHK+23, MT23, SMK+23, ZRR+21, FAB+23]. **optomechanical** [BGK+22, GKN+22, QFA+23]. **orbit** [AAM+20, Iri20, Iri21, KWWZ20, ZS21]. **Orbital** [MMM20, Cin20, LT23, LFRTRP+20, MBKA21, MMM16, Nag20b, NF20, Roy20, SMCNH22, SP20a, TPB+20, GSMT+20]. **orbital-free** [Nag20b]. **orbital-free-related** [LT23]. **Orbital-Specific** [MMM20, Cin20, MMM16]. **orbitals** [GM21, LFRTRP+20, Lom21, SM22, Sha20, SA20, YSZ23]. **orbits** [JVK22]. **Order** [ACM20, AAYA23, ATL+20, ADZA21, Cio22, GXL+22, GML+22, HDF+21, sLLqX+20, PM22, SM22, ZQZ+23a]. **ordered** [FGW+22, RSM+22]. **Ordering** [LYFL21]. **orders** [CPK22]. **Organic** [Üng23, BZW+20, BSS21, BRB+21, FZL+20, HRTSS+20, HW21a, ID21, KPMAB22, KSM+23, KMH+20, KJA+21, LK20, LMAA23, MSKA20, MSKA21, MKuAS+22, MJH+22, NIA21, NLA+21, PIA21, PGPHAPM20, PVR20, PD22, PSJ23, PC22, PNC20, TSW+20, YZW+23, ZZZ+23, ZGCF20]. **organization** [RKG21]. **organocatalysts** [SSIE21]. **organocatalytic** [LLQ+21]. **organophosphorus** [CLL23]. **organosilicon** [HCZ20]. **orientation** [GZCY22]. **Orientations** [BMR21]. **Oriented** [Guh23, WWZ+21, ZYZ+21a]. **origin** [HYY20]. **origins** [GA20]. **ORR** [KS21]. **ortho** [WLH+20, YCSK20]. **ortho-selective** [WLH+20]. **orthogonal** [SD23]. **oscillator** [GN21a, HJIO21, OB21b, TFF+22, WWKH22, YÇDÖ21, TdV21]. **OTf** [TXW+20]. **outer** [GTAL23]. **outer-core** [GTAL23]. **outstanding** [XWLZ20]. **overlap** [GM21]. **oxidation** [CLC+21, ER22, GHZ+23, SKR+21,

SMS23, VGSS20, WXLL21, WWZ+21, XZGS23, YST+21, ZTHW23]. **oxidative** [DYZ+23, ZZZW20]. **oxide** [BTS+21, CYJC20, IMJ21a, IMJ21b, KBR+20, KM21a, LZ23, MI20, MSADA21, MNWD20, RGS23, VN21, ZHFD+20]. **oxides** [KKH21, Kan22, ORL+20a, XWJ+21, YCSK20]. **oximato** [LTC+23]. **oximato-bridged** [LTC+23]. **oximes** [DDSB22]. **oxoiron** [VGSS20]. **oxonium** [KML23]. **oxyethoxy** [ZWL22]. **Oxygen** [CSL+23, CZJ+23, DB20, GKPK21, JJJM21, KS23, PZGH+20, TCL+21, VKS21, XWLZ20, ZTHW23, ZHFD+20]. **oxyl** [SKR+21]. **oxypnictides** [MEWD20]. **ozonolysis** [LWW20].

P [LFRTRP+20, MEWD20, GZC21, RINHY20, WSSD21]. **P-doped** [RINHY20]. **P3CPenT** [PSJ23]. **P3HT** [LMAA23]. **P450** [CS23, QDJY23]. **P450-catalyzed** [QDJY23]. **package** [DGA23, KS22, TJA20]. **packaging** [KS22]. **packet** [Dau21]. **pair** [MHD20, Roy20, VdM22]. **paired** [XgZX+22]. **pairs** [KSPG23, SSIE20]. **pairwise** [RKK+22]. **palladium** [STI20]. **para** [LS21, INV22b]. **para-line** [LS21]. **para}-oligophenylenes** [INV22b]. **paradigm** [RPT21b]. **paradigms** [Mos21]. **Parallel** [GNC20]. **Parameter** [SD23, NLA+21, RPT21a, SSD22]. **Parameterization** [PPR21]. **parameters** [FSR+22, KSM+23, KJA+21, Kha23, Pev21, RRD+22, RPT21b, SIM23, TCSG+20, ZX21]. **paraquat** [HW21b]. **Paratrimerin** [NTND23]. **part** [JJJM21]. **partial** [JBPV21]. **partially** [Ram23]. **Particle** [LRG+20, AJC+21, GRFM20, LMA21]. **Partition** [RĐB+23, TFF+22]. **Partitioning** [CBB21]. **Path** [DKK+20, BM21, CMY22, LYTS20, SMMP+23]. **paths** [SWXM23]. **pathways** [BZW+21, SFPH22, WZL+21]. **patients** [KAA21]. **pattern** [DYG21, ZZZ+23]. **patterns** [CRKMC21, GMRKMCMC21]. **Pauli** [Sah21]. **Pb** [SBKT23, Shi21, XFW+20, KLRS22, KDY+22, LMM+22, MT23, SYD+23]. **PbX** [PAS+21]. **PCBM** [LMAA23]. **Pd** [QOM+20, CZGW22, HLZZ23, SDL+22, ZQZ+23a]. **PdTiZ** [KLRS22]. **PdZn** [LSS+21]. **penalty** [KH20]. **penetration** [XBL23]. **penta** [LZSA20]. **penta-graphene** [LZSA20]. **pentagonal** [RS23, ZMS21]. **pentamer** [MC22, XBK+20]. **pentane** [LZS20]. **pentane-2** [LZS20]. **pentanitrogen** [Mka20]. **pentothal** [CDG+21]. **peptides** [BCLM+22]. **Performance** [MZ21, AAB22, AKKN20, BSS21, BKB+23, CYL+23, CZC+23, EGLJQ+21, FFBH21, HMN20, LK20, LZL+23, LL20, MJH+22, MHS21, NIA21, NLA+21, SUG20, TD22, WLY+20, WWZ+20, WWF23, YZL21a, YCL+22, ZQZ+23a]. **performances** [LXZ+21a, SSIE21, VL21]. **perhalogenated** [SC21]. **periodic** [PGPHAPM20, RS23]. **periodically** [KRB20]. **peripherality** [AD22]. **permutationally** [KKK23]. **perovskite** [AAM+20, BPB+20, LZ20, PSJ23, RMeH+20, RSM+22, SYZF22, ZZLC20, ZCL+22]. **perovskite-type** [RMeH+20]. **perovskites** [FAB+23, KM23, KHK+23, NG20, PAS+21, SMK+23, ZX21]. **peroxidase**

[KI20]. **peroxide** [CSY+21, WWM+22, ZHD+23]. **perspective** [AKP22, GG20a, GG22, KZ21, KMG22, LTC+23, OGT20, PM20, RS21, SIA20, TAS21, XAM+22]. **perspectives** [EPMC20, PAS+21, Sah21]. **perturbation** [AIB21, BMF20, HLL20a, SM22, ZIA20]. **PES** [KK23b]. **PES-Learn's** [KK23b]. **pesticides** [CLL23]. **PEt** [MZ23]. **phase** [BY23, CRC21, CSK21, Dau21, DPC+20, GOS20, GRLH21, HPAM23, HLL20a, KC23, sLLqX+23, LZL+21, ORL+20b, RMLPGHP20, RKI20, SDS19, SDS20, SASA21, Shi21, SG21, VdM22, WXHX22, XZGS23]. **phase-dependent** [Dau21]. **phases** [ARRB+21]. **phenol** [KML23, YST+21]. **Phenyl** [ZXS20, LMAA23]. **phenylazoindoles** [HKM+23]. **phenylene** [CL22, FYL21, LZS20, LMAA23]. **phenylenediamines** [XZGS23]. **phenylenes** [LG22]. **phenylethylammonium** [SYZF22]. **phenylindol** [BSMI23]. **Philicity** [MB23]. **phonon** [PKBZ20]. **phores** [LYT+20]. **phosphide** [fXmTlS+23]. **phosphonic** [FFBH21]. **phosphorene** [CWL+22, GG20a, THL+21, WLY+20, WTC+23, ZHFD+20]. **phosphorous** [RBJ23]. **Phosphorus** [RMB+23, MFE+23, RBJ21]. **phosphorus-doped** [RBJ21]. **phosphorylcholine** [RYC+20]. **photo** [KRA+23, TSN+21]. **photo-detachment** [KRA+23, TSN+21]. **photoassociation** [JWZZ20, Wan21]. **photocatalyst** [RINHY20]. **photocatalytic** [DLZ+21, LYW+20, RHS+21, WLY+20]. **photochemical** [CMM21, TMX+22]. **photoelectron** [GYC20]. **photoelectronic** [XHX+20]. **photoinjection** [MSKA21]. **photon** [BMF20, Dau23, GA20, LXZ+21a, LZ23, SIA21]. **Photophysical** [SFPH22, HMA+22, LMAA23, YLL+20, ZLH20a]. **photosensitizers** [MSKA20, SIA20]. **Photovoltaic** [SIA20, BZW+20, BSS21, FFBH21, FSR+22, GSRG22, JHH+22, KMH+20, KJA+21, LMAA23, RSM+22, XPZ20]. **photovoltaics** [YZW+23]. **phoxim** [CLL23]. **phthalocyanines** [MSA22]. **physical** [RCM+22, RKA+21]. **physico** [RNB22]. **physico-chemical** [RNB22]. **physicochemical** [hHNRA23, KB23]. **physics** [AAAAA23]. **physics-guided** [AAAAA23]. **picture** [JVK22]. **piezoelectric** [MT21]. **piezoelectricity** [SDL+23]. **pilot** [ZMOE23]. **pipeline** [KSM+23]. **pK** [PS23a]. **place** [CLS+22]. **Planar** [ZFB+20, APR20, ILPY+23, KRK+21, TT21a]. **planarity** [Var23]. **plane** [MM20, PS23a, STI20]. **plane-wave** [PS23a]. **plasma** [Bah22, BMF20, CLS+22, KB21, XZGS23]. **plasmas** [DG21]. **plasmon** [UBW+22, KAUB21]. **Plasmonic** [Mok21b]. **Platinum** [PD22, Iri20, Iri21, Üng23]. **Plesset** [HLL20a]. **plus** [NOO+23]. **plutonium** [sLLqX+23, RED21]. **Pn** [MEWD20]. **pnicogen** [ZL21]. **pnictogen** [MEWD20, ZLT+20]. **PNP-catalyzed** [YZD+21]. **point** [LCX+21, PP21]. **points** [BXWK22, HYHW22]. **Poisson** [VL21]. **polar** [BCM+22, MKuAS+22]. **polaritons** [UBW+22]. **polarity** [ADZA21, Hao21, IMJ21b, SN21]. **polarizabilities** [ÉC21, HJL+23, JS21, WP22, YÇDÖ21]. **polarizability** [CBB21]. **Polarizable** [BVL22, RVK23]. **polarization** [Efr23, PM22, STT20, WP22].

polarizing [MT21]. **pollutants** [ARBM21]. **poly** [LMAA23]. **polyacene** [KA21]. **polyaromatic** [LZZW23]. **polyatomic** [BUF+22]. **polyborazines** [LZZW23]. **polychromatic** [TSN+21]. **polycyclic** [Rad21, Var23]. **polymer** [MW21, MJH+22]. **polymerization** [DYK22, MWCJ23]. **polymers** [KK23a]. **polynitrocubane** [LL20]. **polynomial** [CL22, KKK23, SU22]. **polynomials** [HAA+23, SSD22, SD23]. **polyoxometalates** [CSY+21]. **polyoxometalates-supported** [CSY+21]. **polyphenyls** [DL21]. **polysulfide** [AR22]. **polysulfides** [OKK+22]. **polytypes** [ORL+20b]. **POMzites** [VN21]. **Pons** [Yos20]. **Popper** [KHK+23]. **population** [DC22, MKD21]. **pore** [HDF+21]. **porphyrazines** [BWBR21]. **porphyrin** [GMO+20, Üng20, WFG+21]. **porphyrin-** [GMO+20]. **porphyrins** [HLF23, MSA22, MSOA23, Üng20]. **Pöschl** [HJIO21, PMdN21]. **position** [BS20, QFA+23, SSIE20]. **positive** [MOB21]. **positron** [BA22a, STT20]. **positron-electron** [STT20]. **positronium** [HJL+23]. **possible** [AMK+20, Yan20]. **Post** [Var21]. **Post-complete-basis-set** [Var21]. **potassium** [HJIO21]. **Potential** [MC22, MMM20, RK21, TFF+22, ABS20, AIN+20, AB21, BUKA21, BFW+22, BBG20, Dau21, EGLJQ+21, END+23, FWJ+23, FSR+22, GHZ+23, GN20, GN21b, GG20b, HJL+23, HLL20b, IRA+20, JBPV21, JLWH23, KDY+22, KASAK23, Kid21, KH20, KK23b, LFX+21, MSS20, NACP21, NR21, Nat22, NOO+23, OO21a, OO21b, PMGR+21, PMdN21, PJ20b, RS21, RKI20, RR21, SSIE20, SFPH22, SS21, SKG21, STT20, TCL+21, TAMU+23, TD22, XJ20, Yal23, ZGCF20, MM22a]. **potential-based** [JBPV21]. **potentials** [BA22a, BAM20, BCM23, Cin20, Dau23, DFB20, EB22, GN21a, MF21a, MMM16, MZT20, PGROM20, PJ20b, WWKH22, XJLH21, ZYZ+22]. **Povarov** [LLQ+21]. **powder** [FCL22, HYC+21]. **power** [BCM23]. **power-series** [BCM23]. **PPh** [QOM+20]. **PPV** [LMAA23]. **Pr** [SMK+23]. **practical** [KCM+23, Pon19]. **pre** [MSOA23]. **prebiotic** [ES21, SE20]. **precision** [XJLH21]. **predict** [KB23, MSI22]. **predicted** [HMA+22, WJF+21]. **Predicting** [KSM+23, BSMI23, KK23b, PB23]. **Prediction** [ARRB+21, BVL22, HW21a, PP21, Rac21, AAJ+23, BSMB23, BGM+23, FWY+22, GZC21, MRI20, MJH+22, WWL21, WWLL21, WXHX22, Yan21, ZHW23]. **predictions** [GZC21, Jan22, SKR+21, SBG21, SYD+23]. **Predictive** [hHNRA23]. **predictor** [SJ20]. **predominately** [SF20b]. **preference** [FCL22]. **preferred** [CRGD+23]. **Preliminary** [KRS+21]. **prenucleation** [SP20a]. **preorganized** [ÖÇÖ21]. **preparation** [AKP22, SC23]. **prepared** [HPAM23]. **prerequisites** [FMM+23]. **presence** [GN20, GN21b, Hol21, YST+21, ZIA20]. **Pressure** [ONH+21, WXHX22, YCL+22, JSF+21, LWH+21, MIA23, MT21, PJ20a, PKBZ20, Sta21, XFW+20]. **Pressure-induced** [YCL+22, MIA23]. **pressures** [HLL20a, JZX+20, WJF+21]. **prevention** [LS21]. **primary** [WDS+20]. **principle** [HRA+22, KA21, KS21, MIA23, MHS21, MBM+21, PS23a, PS23b, RMeH+20, SMCNH22, TAUM+23, UV20, WXL+21, XFW+20, ZYZ+21b]. **principles**

[AJC+21, AKKN20, CSL+23, CDD23, CZGW22, CWL+22, CZC+23, DLZ+21, ER22, FMH+22, FAB+23, GSRG22, GGUU21, HLZZ23, JZX+20, Kan21, Kan22, KHH+21, KMG22, sLLqX+20, LHZG23, LHL+21, LWH+21, LXWZ21, MBKA21, MSKA21, MAHRA+21, MVF+23, MNWD20, OGSPP+22, Pan20, PL20, RS21, RED21, SFT+21b, SG21, SYD+23, WWM+21, WCM+23, WTC+23, XCZ+21, YZL+21b, ZRR+21, ZLH+20b, tZNb+22]. **prism** [LG22]. **pro** [PGPHAPM20]. **pro-aromatic** [PGPHAPM20]. **probability** [CSS+21]. **probe** [BVL22, ZLH20a]. **probes** [LXZ+21a, LZ23, MF21b]. **Probing** [MSOA23, VM20]. **problems** [LACP21]. **process** [CLC+21, FCL22, MWCJ23, SCZ21]. **processed** [Bah22, KB21]. **processes** [LRG+20, PCEAG23, SMN+23, XZGS23]. **procyanidin** [MWBQ20]. **produce** [LWC+21]. **produced** [ZWW+22]. **product** [Hao21]. **production** [MSS20, SRH20]. **productivity** [SF20b]. **products** [MM22c, SYT+21]. **professors** [BHH20]. **profile** [BSMB23]. **program** [Höf21]. **Projected** [Rui22]. **projection** [Pon19, Yos20]. **projector** [MM22c]. **Promising** [LZ20, FAB+23, KMH+20, RSM+22, WJL+21, XHX+20, YHW+22]. **promoted** [VOK+20, WHYL21, ZZLY22]. **Promoting** [LSS+21, YZD+21]. **promotion** [DRV20]. **propagation** [BSMI23, MSI22]. **propagator** [GRFM20, PM22]. **propargylic** [LLLL20]. **propene** [LZL+23]. **propensity** [BVT20]. **properties** [AAYA23, AMK+20, AAM+20, AIR+23, BA22a, BPB+20, BBAA21, BMF20, BB20, CDD23, CLS+22, CZGW22, CWL+22, CSTD22, CMGH+21, CLLC21, DDSB22, DJC21, DCY21, FWJ+23, FAB+23, FCL22, GXL+22, GML+22, GA20, GRZ+21, GGUU21, HOVG20b, HLL+23, HLZZ23, HMA+22, HNO+21, HFF22, HLF23, HFL23, hHNRA23, INV22b, JZX+20, JZL+21, KB23, KLRS22, KM23, KHH+21, KMH+20, KYL+20, KSP20, KLK21, KMG22, KC23, LLZC20, LCT+22, sLhZX+22, LHZG23, LMA21, LMMA21, LHL+21, LWH+21, LDK23, LFMF23, LMAA23, LZZ+20, MJA20, MZXL21, MKKA21, MKKK22, MKuAS+22, MIA23, MAHRA+21, MGK23, MRI20, MVF+23, MKM+20, Mok21b, MIM21, MBM+21, MSI22, MEWD20, MSCM23, MHG+23, NG20, NR21, NLA+21, NM23, ORL+20a, ONH+21, OMA21, Pan20, PL20, PJ20a, Pan22, PASS21, PB23, PKBZ20, PLZT22, PLT+20, PP23, PP21, RCM+22, RRS21, RKA+21, RNB22, RNH23, RF23, RSM+22]. **properties** [RR21, RMB+23, SIA20, STI20, SAP22, SFPH22, SMP23a, SMP23b, Sha20, dOSdASC+20, SSD22, SG20, SG21, SMK+23, TMH21, UV20, Üng20, WWM+22, WXL+21, WYL22, WJF+21, WXHX22, WCM+23, WOE+22, WTC+23, XPZ20, XFW+20, XCZ+21, XWS+22, YLL+20, YCPW20, YZY+22, YCL+23, YFX+22, ZRR+21, ZLH20a, ZWL22, ZLH+20b, ZZZ20b, ZHFD+20, tZNb+22]. **property** [HZZZ22, PSN23, RNA22, RNB22, TB22, ZXS21]. **propylamine** [SMS23]. **propylene** [CYJC20, CSY+21, WLP+20]. **prospective** [FAB+23]. **prospectus** [SAP22]. **protected** [QOM+20]. **protein** [CP23, GA20, Hol21, KDM+22]. **protein-ligand** [KDM+22]. **Proton** [XBL23, BCLM+22, Dau23, JD20, KML23, NTND23, UHK+22, SE22].

protonated [MZXL21]. **provide** [SMMP+23]. **pseudoharmonic** [GN21a]. **Pseudopotential** [PNC20]. **Pseudopotential-fragment** [PNC20]. **pseudopotentials** [ZMOE23]. **pseudospectral** [ZZJ+23, ZHJ+20]. **Pt** [Iri20, Iri21, QOM+20, RCM+22, Shi21, CZGW22, DLZ+21, MJA20, PPR21, QDC+22, SRH20, XBL23]. **Pt-decorated** [MJA20]. **Pt-supported** [XBL23]. **PtS** [LHZG23]. **Pu** [sLLqX+20, WTC+23]. **puckered** [tZNb+22]. **pulses** [Dau21, GZCY22]. **pure** [JZX+20, XWS+22]. **purely** [MOB21]. **purine** [SE20]. **PVDF** [SK20]. **PVDF-HFP** [SK20]. **PVDF-TrFE** [SK20]. **pyrazine** [HFL23, PGPHAPM20]. **pyrazine-modified** [HFL23]. **pyridine** [WXLL21]. **pyridines** [KPTL23]. **pyrimidine** [YLL+20]. **pyrrole** [PVR20, SCU21]. **pyrroline** [MSADA21]. **pysisyphus** [SKG21]. **Python** [ABS20, GPP+21]. **Python-based** [GPP+21].

QM [CN21, SYL+21, Ram23]. **QM/** [Ram23]. **QM/MM** [CN21, SYL+21]. **QSAR** [BSMI23, KAA21]. **QSPR** [Hav21, KB23, KLT21, KAA21, MSI22, PB23]. **QSPR/QSAR** [KAA21]. **QTAIM** [LFMG20, NYX+22]. **QTAIM/IQA** [LFMG20]. **quadrilateral** [FLZP23]. **Qualitative** [TLT+22]. **Quality** [hHRN+23]. **quantification** [KDM+22]. **Quantitative** [HZZZ22, JPSC20, RNA22, RNB22, RNH23, TB22, TLT+22]. **Quantum** [BM21, CSK21, GB21, GM21, KA23, KDM+22, MJA20, MJRS20, NZ20, NOO+23, ORL+20a, RBSW21b, SBM22, SBKT23, SD20, Sta21, VOK+20, WP20, AkAR+21, AKP22, BHN23, BU20, BUKA21, Bah22, BMF20, BCLM+22, BWR22, BRF21, CDD23, CWW+23, CM21, Cio22, CJVF+23, Cla22, CLLC21, DKK+20, Dau21, DGA23, FAB+23, GKN+22, GG20a, GN21a, GPP+21, GDR21, GTC+23, HPAM23, HHA23, HHG+21, HCZ20, HZC21, IRA+20, KB21, Kön21, KS22, KK23b, KCM+23, LACP21, LC20, LRG+20, LLC20, MM22c, MFK22, Mok21a, MAMB+22, MIM21, MB23, MSI22, Mos21, MSCM23, NHNO20, Nat22, Ole20, Ole21, OMA21, RMM+22, RKK+22, RBJ23, RKI20, SDS19, SDS20, SI20, Sha20, SUG20, SMS23, SC23, Sur20, Sur22, TFF+22, UHK+22, VKS21, WWL21, WAM+20, XgZX+22, XWS+22, YCL+23, ZMOE23, ZMJ+20, ZHW23]. **Quantum** [SRH20]. **Quantum-chemical** [GB21, SBM22, VOK+20]. **Quantum-classical** [BM21]. **Quantum-phase** [CSK21]. **quartet** [NdVVT22]. **quartic** [OB21b, TdV21]. **quasi** [Var23]. **quasi-molecule** [Var23]. **quaternary** [AIR+23, LMM+22, Rac21, WWLL21]. **quaterthiophene** [SV21]. **Qubit** [XgZX+22]. **quest** [Var21]. **question** [HKM+23]. **quinoline** [MVF+23, ZLG22].

R [YCSK20]. **R1216** [LZL+23]. **Radial** [ZHJ+20, PMGR+21, ZZJ+23]. **radiated** [SBG21]. **radiation** [JAZ+20]. **Radiative** [TSHRS+20]. **radical** [ASO+22, BVT20, DYK22, FMG23, KML23, SRS21, SYT+21, SXTZ23, YST+21, ZWZB23]. **radical-scavenging** [BVT20]. **radicals** [CLW21, DFK20, DYK22, JAZ+20, SCZ21, SMS23]. **radii** [LYFL21].

rainbow [Jan22]. **Raman** [FPdS21]. **Randić** [BMR21]. **random** [FYL21, LSG21, LGW23]. **range** [EB22, KA21, PT21]. **Rank** [CL21]. **Rao** [EAPCD21]. **Rapid** [ÖÇÖ21]. **rare** [MBKA21, NG20]. **rare-earth-based** [NG20]. **rasagiline** [RGLG23]. **rate** [CZW21]. **rates** [BM21]. **ratio** [Nat22]. **rational** [LSA+22]. **ray** [BWBR21, HP21, MSOA23, RG20]. **Rb** [RMeH+20, AMK+20, FAB+23, GSRG22]. **RDkit** [KSM+23]. **RDX** [MWC+21]. **Re** [KWWZ20, SMK+23, PJ20a, SMK+23]. **Reaction** [TSS+23, ASO+22, BZP+20, BM21, BTS+21, CMY22, CLL23, CSY+21, CMM+22, DYZ+23, dSFdSdMdM20, GKPK21, HW21b, JWZZ20, JD20, KZ21, KWWZ20, KV23, KS23, LLX+23, SMMP+23, SXTZ23, TCL+21, VKS21, VKK+21, WWM+22, WY20, WZL+21, WWZ+21, WCZ+20, YYL21, ZZZ+20a, ZHD+23, ZHS21]. **Reactions** [DFK20, ABDD22, CMM21, CZJ+23, CBK+20, ES21, HH23, HCZ20, LLQ+21, MSADA21, MAMB+22, QdOdMC+21, RRSF22, SMMP+23, SBM22, SE20, SMS23, TPB+20, UHK+22, UAH+20, VOK+20]. **reactive** [HBY20]. **Reactivity** [DYK22, CMM+22, KLT21, LWC+21, LZZW23, LLMQ20, MB23, SMCNH22, SMMP+23]. **Reagent** [LLZ+20, KAG+20]. **real** [KVCS21]. **real-time** [KVCS21]. **rearrangement** [LFMG20, XBK+20]. **ReaxFF** [TCL+21, TCX+22]. **ReaxFF-based** [TCL+21, TCX+22]. **receiver** [SV21]. **recombination** [BZW+20]. **recurrence** [GM21]. **recursive** [UR23]. **redox** [HW21b, ZYZ+22]. **Reduced** [DS20, ATL+20, BMH21, Cio22, MPBL23, Ram23]. **reduction** [CSL+23, CZJ+23, EB22, GKPK21, KS23, LXWZ21, MSM+20, RR21, SSIE20, VKS21, XQJ+21, KA23]. **reference** [Eti20, HPAM23, JBPV21, MKD21, dLRdLJ+20]. **reflecting** [KRA+23]. **reforming** [RSD21]. **Regio** [MF21b]. **region** [WZ21]. **regioselective** [WSSD21]. **Regioselectivity** [QDJY23]. **regression** [AGK23, BSMI23, GZC21, MSI22]. **regular** [DQS+21]. **Regulating** [GRZ+21, WWZ+21]. **reinvestigation** [LWW20]. **related** [IMJ21b, LT23, SBKT23]. **Relating** [RRD+22]. **relation** [LZS20]. **relations** [GM21, JMOW20]. **relationship** [AA23, CMM+22, HZZZ22, JPSC20, LDS+23, LZZW23, RNA22, RNB22, RNH23, TB22, YCSK20]. **Relative** [Nag20b]. **Relativistic** [AKK+21, AMM21, JVK22, OAJ21, HOVG20b, HTNP21, KSP20, MSS22, MZT20, Nan23, OGT20, PT21, QOM+20, SPR22, XJLH21, ZMOE23]. **relaxation** [CZW21, INV22b]. **release** [Roy20]. **relevant** [HBY20]. **reliable** [KLT21]. **remarkable** [XHX+20]. **Remarks** [Ali20]. **remdesivir** [FMS+22, LS21]. **removal** [FAJOF20]. **remove** [ZQZ+23b]. **Renner** [KRS+21, MM20]. **renormalization** [TT21b]. **Rényi** [GN21b, Nat22, Ole20]. **reorganization** [SPF+22]. **replacement** [Pev21]. **Reply** [MMM20, OO21b]. **reporting** [WV21]. **representation** [AB21, DS20, WP22]. **Representations** [RC20, CM21, RP22]. **representing** [TLL23]. **reproducible** [GKK21]. **repurposed** [LAAP21]. **research** [BHH20, Nag20a, SF20b, Shi20]. **residues** [BESG22]. **resistance** [NYX+21].

Resonance [JBPV21, OAJ21]. **resonances** [BAM20, CWW+23]. **resonant** [WZ21]. **respect** [FLZP23]. **Response** [OB21a, Tak22b, AMM21, Bah22, BMF20, DS20, GRZ+21, HP21, HDF+21, KB21, LZS20, OR21, PM22, QFA+23, Rac21, RMS+23, STN20, Tak22a, UP20, ZAB+23, ZZLC20]. **responses** [GUUG23, TSW+20]. **responsivity** [YXKJ21]. **REST** [HHG+21]. **restrained** [ABS20]. **restricted** [GSMT+20, GOT+23]. **retrochalcones** [MK21]. **reveal** [Cio22]. **revealed** [AKKN20]. **Revealing** [GUUG23, DYZ+23]. **Reverse** [Cio22, AGK23, LYTS20]. **reversible** [ZHG+22]. **Review** [BRB+21, EM21, YST+21, AB21, Doh20, HHA23, LRG+20, MP20, RMM+22, SBM22, SC23]. **revisited** [BCKN21, CMY22, Sør21]. **Revisiting** [APR20, KKK23, ZZJ+23, ZHJ+20]. **Rh** [CZGW22, GGUU21, HLZZ23, LWR21, ZZZW20]. **Rh-catalyzed** [LWR21, ZZZW20]. **rhodamine** [LXZ+21a]. **rhodamine-contained** [LXZ+21a]. **rhodium** [WSSD21, WLH+20, YYL21]. **rhodium-catalyzed** [WSSD21, YYL21]. **rich** [HNO+21, MZ21, ZJW+21, ZYZ+21b]. **rigid** [CWY+20]. **ring** [BS20, CYJC20, dSFdSdMdM20, KDY+22, LNC+23, MW21, MWCJ23, MAMB+22, PM20, RĐB+23, SWXM23, Tia21, YLL+20, ZAB+23, ZFB+20, ZZL+20a]. **ring-opening** [dSFdSdMdM20, MWCJ23, MAMB+22]. **rings** [dSFdSdMdM20, PVR20, Rad21]. **Ritz** [SBA21]. **RMX** [PLT+20]. **Rn** [dAOdASP+20]. **Ro** [NR21, JVK22]. **Ro-vibrational** [NR21, JVK22]. **roadmap** [VN21]. **Robustness** [SG21]. **Role** [LFRTRP+20, SPF+22, BRF21, CMGH+21, GRLH21, HMA+22, HFF22, MFK22, PGPHAPM20]. **ronidazole** [CXZ+21]. **roots** [BXWK22]. **Rosen** [BU20]. **rosettes** [PS22]. **rotary** [WAM+20]. **rotating** [SS21]. **Rotation** [HJIO21, HKM+23]. **rotational** [WY20, Wan21]. **rotational-excited** [WY20]. **rotaxane** [BS20]. **rotor** [CWY+20]. **route** [CLW21, Kön21, MSS20]. **rovibronic** [HSV22]. **row** [BHN23, JXM22, RNFMC20]. **RPA** [JS21]. **Ru** [RCM+22, RR21, BB20, CZGW22, HLZZ23, PJ20a]. **Ruddlesden** [KHK+23]. **rules** [AS22, XHS+23]. **running** [HHA23]. **RuPtSb** [RCM+22]. **ruthenium** [Kid21, RR21, SCAD+20]. **rutile** [DK21].

S [CSL+23, EGLJQ+21, EB22, PASS21, PPCF+20, SPF+22, WAM+20, ZFB+20, NYX+21, dAOdASP+20, OKK+22, PLZT22, RS23, SK21, SPR21, SPR22, WAM+20]. **saddle** [BXWK22]. **Salen** [UBV+21, CYJC20, RR21]. **salt** [Yan20]. **salts** [HDF+21]. **same** [Rui22]. **sandwich** [DLZ+21, KDY+22, YZY+22]. **saturated** [HZZZ22, UIIP23]. **Sb** [BB20, KMG22, MEWD20, Yan20, EGLJQ+21, SG22]. **scalar** [KSP20, XAM+22]. **scale** [ISL+23, SIA20, UBV+21, ZMJ+20]. **scales** [MB23]. **scaling** [CJVF+23]. **Scandium** [CMGH+21]. **scattering** [BA22a, BA22b, KK23b, MSS22, SDK+21]. **scavenging** [BVT20]. **scented** [FMG23]. **SCF** [JXM22]. **ScGe** [WYL22]. **scheme** [KV23, LFRTRP+20, VKK+21]. **Schiff** [GG20b]. **Schrodinger** [SS21, HRA+22, LBP20, Sah21, SD20]. **Schultz** [LGW23]. **Schwarz**

[ZZJ+23]. **Schwarz-like** [ZZJ+23]. **Science** [GG22, MNN+20, SC23]. **Sciences** [MNN+20]. **ScK** [AJC+21]. **scores** [BGM+23]. **screened** [AIN+20, HJL+23, MF21a, SDS19, SDS20, WKH20, WWKH22, XJLH21]. **screened-hydrogenlike** [WKH20]. **screening** [JXL+21, KPMAB22, dOSdASC+20, WJL+21, ZJW+21]. **screw** [BU20]. **ScYH** [WJF+21]. **Se** [EB22, PASS21, SPF+22]. **seams** [Xav23]. **search** [KRK+21, KYL+20, KAG+20, MJH+22, ZFB+20]. **Searching** [BESG22, RGLG23]. **second** [AAYA23, ATL+20, ADZA21, GXL+22, GML+22, HDF+21, NF20, RNFMC20, SM22]. **second-order** [AAYA23, ATL+20, GXL+22, GML+22, HDF+21, SM22]. **secondary** [AS22]. **sections** [MW21]. **segregation** [WWM+21]. **Selected** [SSK20, KML23]. **selection** [XHS+23]. **Selective** [LNC+23, SRH20, HRTSS+20, LSS+21, MW21, STF21, WLH+20]. **selectivity** [GG20a, JRA21, LZ21]. **selenide** [AAB22]. **selenides** [AIR+23]. **selenium** [RMLPGHP20]. **Self** [ES21, SE20, SLdS20, Eti20, HK22, HP21, PS22, SM22]. **self-assembled** [PS22]. **Self-catalytic** [ES21, SE20]. **Self-catalyzed** [SLdS20]. **self-consistent** [HK22, HP21, SM22]. **self-contained** [Eti20]. **semiclassical** [ZHS21]. **semiconducting** [Mok21a, NIA21]. **semiconductor** [CDD23, DCY21]. **semiconductors** [MMP23]. **semiempirical** [WWL21]. **Sensing** [CWL+22, HRTSS+20, LXZ+21a, MJA20, NHH22, PLZT22, SCY+23, THS20, TSHRS+20, dPZFM+22]. **sensitivity** [GG20a]. **sensitization** [GG20b]. **Sensitized** [SSS23, FFBH21, FZL+20, MSKA20, PIA21, PGPHAPM20]. **sensitizers** [SSS23]. **sensor** [GG20a]. **separation** [LNC+23, MJRS20]. **sequence** [LLZ+20, NdVVT22, TVdVN22]. **sequences** [NdVVT22, TVdVN21, TVdVN22]. **sequestration** [QdOdMC+21]. **series** [AkAR+21, BCM23, GZWL22, GTC+23, JXL+21, LMM+22, MAMB+22, WZ20, ZPS+20]. **SeS** [tZNb+22]. **set** [Ale23, BT23, Cha21b, DK21, HMBPJ+20, QdOdMC+21, STI20, SM22, SK21, Var21]. **sets** [GSMT+20, KCM+23, NLA+21, RPT21a, VP20]. **setting** [RPT21a]. **several** [SWXM23]. **sexipyridine** [ZXS21]. **SGS** [SG22]. **SH** [BZP+20]. **Shannon** [AIN+20, SJ20, SLPS20, TPCSD20]. **Shannon-information** [SLPS20]. **shape** [FPdS21, HSV22, KMH+20]. **shaped** [PMdN21]. **shapes** [GZCY22]. **shared** [TPB+20]. **shared-orbital** [TPB+20]. **sheets** [ARBM21]. **shell** [Fin21, ZZJ+23]. **shell-confined** [ZZJ+23]. **shells** [SBKT23]. **shielding** [CRKMC21, HMN20, OAJ21]. **shieldings** [VCM+21]. **shift** [GZC21, GMRKMCMC21, HMN20]. **Shifts** [Cha21a, SK21]. **Short** [PT21, DYK22]. **Short-range** [PT21]. **Should** [RBSW21b]. **show** [PZGH+20]. **Si** [CZGW22, GZWL22, GUUG23, GTC+23, ILPY+23, KDY+22, LMM+22, NHH22, VKS21, tZNb+22]. **Si-doped** [NHH22, VKS21]. **SiB** [PP21]. **SiC** [LFX+21, TEEH23]. **side** [LC20]. **SiF** [FAB+23]. **significant** [PZGH+20]. **signless** [LXZ21b]. **silanes** [SC21]. **silanol** [CSY+21]. **silanol-functionalized** [CSY+21]. **silica** [UBW+22]. **silicene**

[Mok21c]. **silicide** [GZWL22]. **silicides** [CZGW22]. **silico** [JPSC20, KRK+21, LZ23, MYS23, PRC23]. **silicon** [DYG21, FMH+22, GYC20, KRK+21, MKKK22, ZZZ20b]. **silol** [XPZ20]. **silver** [HFL23, Ram23, UBW+22]. **SiMg** [ZZZ20b]. **similar** [Hao21]. **similarity** [GN21a, Izs21, MB23]. **Simon** [Ano22a]. **simple** [ACM20, P´23, THS20, WZ20, ZWW+22]. **Simplified** [GSMT+20]. **simulated** [TSN+21]. **Simulating** [HP21]. **simulation** [CS23, CSTD22, DFB20, JAZ+20, MWC+21, TCX+22]. **simulations** [DKK+20, Doh20, HHA23, KPMAB22, LCH+22, MZD+20, PP23, ZL23, ZLG22]. **Simultaneous** [MOB21, LFMG20, Xav23]. **sine** [SS21]. **Single** [GM21, VKS21, AR22, CSL+23, CZJ+23, DLZ+21, Eti20, LLX+23, SMP23a, TSS+23, XgZX+22]. **single-atom** [AR22, CSL+23, DLZ+21]. **Single-Center** [GM21]. **single-reference** [Eti20]. **single-walled** [SMP23a]. **singles** [BBG20, dSFdSdMdM20]. **singlet** [CPK22, JJJM21, LYTS20, TAUM+23, TVdVN22]. **singlet-state** [CPK22]. **singlet-triplet** [TAUM+23]. **singly** [KKH21]. **SiO** [WLP+20, AII21, LCY+23, MAK+22]. **Site** [sLLqX+23, KKK23]. **Site-dependent** [sLLqX+23]. **sites** [CPL+21, DTAS21, GKPK21]. **six** [JRA21, ZZL+20a]. **six-membered** [ZZL+20a]. **Size** [FPdS21, HDF+21]. **sized** [GW21]. **skin** [GG20b]. **skutterudite** [KMG22]. **Slater** [GM21, BKB+23, NZ20, YSZ23]. **Slater-Type** [GM21, YSZ23]. **Slow** [BGK+22, CWW+23]. **Sm** [SMK+23]. **small** [AMM21, GW21, HFL23, KPMAB22, KJA+21, LAKJ20, ÖÇÖ21, ZMOE23]. **small-core** [ZMOE23]. **small-molecule** [ÖÇÖ21]. **small-sized** [GW21]. **smallest** [ZFB+20]. **SmFeO** [MT21]. **Sn** [LYPD23, GUUG23, LMM+22, SYD+23]. **SnC** [TEEH23]. **SnI** [RSM+22]. **SnO** [AAJ+23]. **SOA** [RKA+21]. **sodium** [CDG+21, EGLJQ+21]. **sodium-ion** [EGLJQ+21]. **SOF** [PLZT22]. **soft** [BA22b]. **Software** [MNN+20, DGA23, KS22, TJA20]. **Solar** [SSS23, BSS21, FFBH21, FZL+20, JHH+22, KPMAB22, KMH+20, KJA+21, LZ20, MSKA20, MJH+22, PIA21, PGPHAPM20, PSJ23, SIA20, ZZZ+23]. **solar-cells** [PGPHAPM20]. **solid** [CZ21, HLL20a, SBG21]. **solitons** [PMdN21]. **sols** [LLW+21]. **solution** [Doh20, HW21b, KMK21, KK21, KLK21, P´23, SS21]. **solutions** [CWY+20, GN20, PGROM20, RED21, WV21]. **Solvation** [MHD20, BY23, OKK+22, RR21]. **Solvent** [HW21b, HOVG20b, MSM+20, OAJ21, QdOdMC+21, TPT20]. **Solvent-dependent** [HW21b]. **solvents** [MKuAS+22, ZYZ+22, ZGCF20]. **Sombor** [DTW21, FYL21, LCX+21, LGW23]. **some** [AN20, AIAG21, FYL21, dSFdSdMdM20, GSMT+20, Hao21, Hav21, KAA21, LC20, LGW23, MK21, MP20, TB22, Üng23]. **SOPPA** [JS21]. **sound** [YFX+22]. **space** [ATL+20, BBTN23, CN21, HP21, JBPV21, MBR21a, SMN+23]. **spacers** [SSS23]. **spaces** [KRB20, WFG+21]. **spacing** [NM23]. **spanning** [LG22].

Spatial [RPT21b, ZZ22]. **Spatially** [GSMT+20, MR21]. **Special** [Ano20-47, KKRR21, WZ21]. **species** [Bra21, KRK+21, MM21, SMN+23]. **Specific** [MMM20, Cin20, MMM16]. **specifications** [BU20]. **spectra** [BWBR21, HP21, Jan22, KASAK23, Kön21, LNE+20, LDK23, MEBL22, MSOA23, RRSF22, SSK20, SN21, WOE+22]. **spectral** [BRB+21, CLS+22, LYFL21, UP20, ZZZ20b]. **spectroscopic** [BY23, CRGD+23]. **spectroscopy** [BWR22, FPdS21, GKPK21, GNC20, GYC20, KPTL23, dAOdASP+20, PNC20, RYC+20, TLT+22]. **spectrum** [GN20, HJIO21, INV22b, JD20, KK21, KLK21, LG22, MFC20b, STT20]. **sphere** [MR21]. **spherical** [TAUM+23, YÇDÖ21]. **spherically** [HJL+23]. **Spin** [SBAT23, AMRS22, AAM+20, CSK21, CM21, Iri20, Iri21, KWWZ20, KGSD20, KPTL23, MSOA23, Pon19, RR21, SY21, TWT+21, TPB+20, TVdVN22, UR23, VGSS20, Yos20, ZS21, NdVVT22, TVdVN22]. **spin-adapted** [UR23]. **spin-adiabatic** [TPB+20]. **spin-coupled** [SY21]. **spin-crossing** [TPB+20]. **spin-crossover** [KPTL23]. **spin-orbit** [ZS21]. **Spin-quartet** [NdVVT22]. **Spin-singlet** [TVdVN22]. **spin-state** [KGSD20]. **Spin-tautomery** [SBAT23]. **spin-triplet** [TVdVN22]. **spinel** [MHG+23, ORL+20a]. **spinterface** [MKM+20]. **spintronic** [AMK+20, MMP23, MTA+22, SG22, SMP23b, TMH21]. **spintronics** [Rac21]. **spirobi** [GB21]. **spirobifullerene** [KMH+20]. **Splitting** [DTAS21, LYW+20, SSIE20, ZHJ+20]. **squared** [NOO+23]. **squares** [PJ20b]. **Sr** [PZGH+20, Tia21, XFW+20, KHK+23, PZGH+20, VCM+21]. **SrO** [FPdS21]. **stabilities** [XHX+20, ZRR+21]. **Stability** [DG21, LFMF23, AN20, BSS21, CP23, DYG21, FAX+23, FPdS21, GW21, GYC20, JZL+21, LYPD23, PJ20a, PSN23, PMdN21, PP23, PS23b, Ram23, RSD21, SDS19, SDS20, SBJ20, SG21, SYD+23, VdM22, WWM+21, WXHX22, WCM+23, ZLH+20b, ZZZ20b]. **Stabilization** [WWWC21]. **stabilized** [Guh23]. **stable** [PAS+21, SZMM22, ZMS21]. **stacked** [Mok21c]. **stacking** [ZZZ+23]. **stage** [KYL+20]. **stages** [DYK22]. **standard** [GSMT+20, WWL21]. **standing** [HZC21]. **Stark** [BAM20]. **State** [AKP22, MW21, ACM20, BXWK22, CZ21, CZW21, CPK22, DSNZ+20, Eti20, HPAM23, KGSD20, KYL+20, LFRTRP+20, LHL+21, NdVVT22, Nag20b, NZ20, NZAH21, NTND23, NYX+21, PGROM20, Rui22, SV21, SPR21, SC23, TSN+21, TVdVN21, UHK+22, Yal23, ZHS21]. **state-natural** [LFRTRP+20]. **State-selective** [MW21]. **states** [AMRS22, CPL+21, DFB20, GDR21, Izs21, KK21, sLhZX+22, LBG20, Mka20, MM21, MSOA23, NHNO20, Nat22, RR21, Rui22, SBG21, SPR22, SKG21, TWT+21, TPB+20, TPCSD20, TT21b, TVdVN22, VGSS20, VNK+23, WY20, WWKH22, Xav23, YÇDÖ21, dLRdLJ+20]. **static** [NHNO20, SFB20]. **stationary** [TLL23]. **Statistical** [LMMA21, Pev21]. **steel** [DPC+20]. **Steiner** [RMWF20]. **step** [KA23, LFMG20, WCZ+20]. **stepwise** [HH23, KZ21, WCZ+20]. **Stereo** [HYHW22]. **Stereo-dependent** [HYHW22]. **stereochemical** [MF21b]. **Stereochemistry** [MFE+23]. **Stereodynamics** [WY20]. **stereoselectivity** [TXW+20]. **steric**

[SC21, YCSK20]. **stoichiometric** [MSM+20]. **storage** [DRV20, KDY+22, KHH+21, LFX+21, RS21, RKA+21, RMeH+20, SNL+23, TEEH23, YZL21a, ZHG+22]. **Strain** [LLZC20, RSM+22, tZNb+22, HLL+23, LHZG23, LXWZ21, WLY+20, YCPW20]. **Strain-tunable** [LLZC20]. **strained** [GMRKMCMC21, SC21]. **Strangely** [GOR20]. **strength** [AA23, BVL22, LAKJ20, sLLqX+23, ZZF22]. **strengths** [WWKH22, YÇDÖ21]. **stress** [MAMB+22]. **strip** [QSZ23]. **Strong** [Dau23, Dau21, LG22]. **Strong-field** [Dau23]. **Structural** [GYC20, HFL23, JZX+20, JZL+21, KHH+21, LYPD23, LWH+21, MAHRA+21, MBM+21, MHG+23, NLA+21, PLT+20, RMM+22, SUSS23, SYD+23, fXmTlS+23, AAM+20, AS22, AKK+21, BSS21, BB20, CMGH+21, DYG21, FAB+23, HNO+21, HBY20, KLRS22, KHK+23, KMG22, KC23, LTC+23, MSKA20, MKKA21, MKuAS+22, MK21, MIM21, MNWD20, MEWD20, NM23, ORL+20a, Pan20, PJ20a, Pan22, RPAA22, SMP23a, SUG20, SG20, TCSG+20, XFW+20, ZRR+21, tZNb+22]. **Structure** [BWLZ22, Kov20, LZZW23, MGK23, YCSK20, AN20, AJC+21, BRB+21, BWBR21, CSY+21, CMM+22, DDSB22, Doh20, DLZ+21, EM21, FMS+22, FPdS21, FH21, GNC20, GXL+22, Gun21, HLL20a, HLL+23, HLZZ23, HZZZ22, INEB23, JPSC20, KKH21, Kön21, LLW+21, LDS+23, LFMF23, MZD+20, MA23, PP21, RRD+22, RNA22, RNB22, RNH23, RNFMC20, RKG21, SBA21, SBJ20, TB22, WXL+21, WWM+21, WYL22, WP20, WFG+21, XBK+20, ZGCF20, ZHJ+20, ZMS21, tZNb+22, PP23]. **Structure-activity** [YCSK20]. **Structure-aromaticity-reactivity** [LZZW23]. **Structure-dependence** [BWLZ22]. **structure-properties** [RNH23]. **structure-property** [HZZZ22, RNA22, RNB22]. **structure-reactivity** [CMM+22]. **structure-toxicity** [JPSC20]. **Structures** [JAZ+20, LCT+22, VCM+21, DCY21, ELH20, HAA+23, IAI20, KYL+20, LSG21, Nan23, PZGH+20, ÜB20, WZ21, ZG21, ZZZ20b, ZZL20b]. **Strychnos** [SSK20]. **students** [BHH20, CM21]. **studied** [sLLqX+20, MZD+20, ORL+20b]. **Studies** [GOT+23, AAN+21, AMRS22, BRB+21, CYJC20, GG20b, KLT21, LZL+23, SSEI21, SPR22, TCL+21, WWZ+20, WWM+21, WAW+21, XPZ20, XHX+20, ZL21]. **Study** [FWJ+23, JXYL20, LZSA20, MM21, SCY+23, ZL23, AAJ+23, AAYA23, AAM+20, ASO+22, AR22, ABDD22, BY23, BHN23, BBAA21, BMF20, BZP+20, BZW+21, BCLM+22, BB20, Bra21, BSH+21, CCZ20, CZ21, CWL+22, CLL23, CZC+23, CMGH+21, CPL+21, CMM+22, DRV20, DPC+20, DYJ+22, DFK20, DLZ+21, FFBH21, FK20, FMH+22, FGW+22, dSFdSdMdM20, FMM+23, GB21, GHZ+23, GTAL23, GNC20, GGUU21, HAA+23, HTNP21, HLZZ23, HLF23, HFL23, HZC21, INV22b, ISL+23, JPSC20, JBPV21, JAZ+20, JZX+20, JSF+21, JWZZ20, KLRS22, KBR+20, KHH+21, KHK+23, KVCS21, Kha23, KS21, LK20, LLLL20, LLW+21, LK21, LZ21, LG21, LCT+22, sLsHtW+23, LNC+23, LHZG23, LLX+23, LWR21, LSS+21, MJA20, MZXL21, MSS22, MKKA21, MBKA21, MSKA21, MKKK22, MR21, MZF21, MIA23, MAHRA+21, MVF+23, MWCJ23, MI20, Mka20,

MSADA21, MIM21, MM20, MHS21, MPBL23, MBM+21, MT21, MSCM23]. **study** [MHG+23, NZ20, NTND23, dAOdASP+20, PASS21, PSJ22, PSN23, PGPHAPM20, PD22, PRC23, RMS+23, RS23, RBJ23, RINHY20, RSD21, RKG21, RC20, RED21, SPF+22, SFPH22, SBM22, SMP23a, SWXM23, SU22, SDL+22, SNL+23, Shi21, SG20, SMS23, SRS21, STF21, SYT+21, SXTZ23, TSN+21, TXW+20, THL+21, TLT+22, TSW+20, TMX+22, ÜB20, VSKG21, WLP+20, WZ20, WV20b, WXL+21, WCM+23, WLH+20, WHYL21, WTC+23, XZ20, XQJ+21, XCZ+21, XWS+22, XZGS23, YZW+23, YZD+21, YCL+23, YZL+21b, YHW+22, YHZ+22, ZIA20, ZZZW20, ZZZ+20a, ZLT+20, ZLH20a, ZZLC20, ZXS21, ZTHW23, ZHD+23, ZKP22, ZZZ20b, ZZLY22, ZHS21, dLRdLJ+20, tZNb+22, TEEH23, YST+21]. **studying** [SC21]. **styryl** [TPT20]. **styryl-bodipy** [TPT20]. **sub** [ISL+23, SMN+23]. **sub-Hilbert** [SMN+23]. **sub-nanometer** [ISL+23]. **Subfemtosecond** [Mok21c]. **subjected** [Mok21a, NR21]. **subphthalocyanine** [CCZ20]. **subphthalocyanine-AzaBODIPY-C** [CCZ20]. **subsequent** [AAN+21, SYT+21]. **Substantial** [AAYA23]. **Substituent** [HLL20b, SSEI21, PCEAG23, UIIP23, WLLS21, YCSK20]. **substituents** [BA21, DSNZ+20, HMA+22, LYT+20, PVR20]. **substitute** [YHW+22]. **substituted** [KM21b, SWML23, ZXS20]. **substitution** [AAB22, CLL20, MT23, MEWD20, SSIE20, ZL21]. **subsystem** [GTV20, STN20]. **subsystem-based** [STN20]. **subsystems** [MJRS20]. **subunits** [TD22]. **success** [Shi20]. **sufficient** [Sør21]. **sugar** [ZWW+22]. **suitable** [KJA+21, Pev21, SG22]. **sulfide** [FCL22, RDMF21]. **sulfolane** [OKK+22]. **sulfonylimino** [NHNO20]. **sulfonylimino-** [NHNO20]. **sulfonyltriazoles** [WLH+20]. **Sulfur** [ZYZ+21b, CSL+23, MZF21, THS20]. **sulfur-doped** [THS20]. **sulfur-functionalized** [CSL+23]. **sulfuric** [WCZ+20]. **sulphide** [dAOdASP+20]. **sum** [SLPS20]. **sums** [KRB20]. **superacids** [PVR20]. **superalkali** [HDF+21]. **superatom** [LWC+21]. **Superatomic** [Ari21, Yan21]. **superatoms** [QOM+20]. **superbasic** [VOK+20]. **supercapacitors** [XWS+22]. **superconducting** [WJF+21]. **superheavy** [MZT20]. **superphenalene** [RPAA22]. **superposition** [DK21, SM22]. **superradiant** [CRC21]. **supertriphenylene** [RPAA22]. **supported** [CSL+23, CSY+21, DLZ+21, LLX+23, VSKG21, WWM+22, XBL23]. **Supramolecular** [SN21, CCZ20, RKG21]. **surface** [BFW+22, BSMB23, CXZ+21, KRA+23, KK23b, LRG+20, LQZ+21, MC22, RHS+21, RK21, UBW+22, YZL+21b, ZL23]. **surfaces** [DB20, HYY20, KKK23, MBR21a, RKI20, SKG21]. **Sustainable** [KS22]. **SVECV** [KV23, VKK+21]. **SVECV-f12** [KV23, VKK+21]. **SVPD** [TCSG+20]. **swap** [YCL+23]. **swarm** [AJC+21]. **switch** [BMH21]. **switchable** [BS20]. **Symmetry** [MSCM23, AIB21, BA22a, Rui22, ZZ22]. **symmetry-adapted** [AIB21]. **synergistic** [JHH+22, LXWZ21]. **synthesis** [CDG+21, LL20, SWML23]. **synthesize** [Yan20]. **synthesized** [Üng23]. **system**

[AkAR+21, BGK+22, CWW+23, CZW21, FMS+22, GKN+22, KGSD20, MM20, OKK+22, PSJ22, QFA+23, SDS19, SDS20, YCL+22, ZFB+20, GG22]. **system-** [MM20]. **systematic** [GZC21, HMBPJ+20, KHK+23]. **systems** [AB21, BBTN23, CRC21, CFJ20, Cha21b, CL22, CSK21, CDR20, CSGR21, Gun21, Hua20, KZ21, Kön21, Lom21, PJ20b, RC20, SF20a, SPR22, SD20, TAMU+23, VOK+20, Wan21, ZIA20]. **Szeged** [Ano22a, BT21, IMJ21a, LC23]. **Szeged-like** [Ano22a, BT21]. **Szeged-type** [IMJ21a].

T [BT23, LZZ+20, VNK+23]. **Tailored** [Kön21, SG20]. **tailoring** [BA21, YZL21a]. **taking** [CLS+22]. **tautomeric** [EM21]. **Tautomerism** [SE22, KMK21, LZS20]. **tautomerization** [SLdS20]. **tautomery** [SBAT23]. **TaZ** [AMK+20]. **TbSi** [GYC20]. **TD** [CMM21, HMA+22, KLK21, MEBL22, PGPHAPM20]. **TD-DFT** [CMM21, KLK21, PGPHAPM20, HMA+22, MEBL22]. **TD-DFT/periodic** [PGPHAPM20]. **TDDFT** [XZ20]. **Te** [PASS21, WLLS21]. **teaching** [CM21]. **technique** [SBA21]. **techniques** [BSMI23, BGM+23]. **Technology** [GG22, HHA23, SG22]. **Teller** [HJIO21, HL20, KRS+21, MM20, PMdN21]. **tellurium** [KI20, RMLPGHP20]. **tellurium-based** [KI20]. **Temperature** [sLhZX+22, ORL+20b, BCM23, GTC+23, HZZZ22, Rac21, SMP23b, WCM+23]. **Temperature-dependent** [sLhZX+22, GTC+23]. **temperatures** [HLL20a, SDL+23, WV20b]. **tempering** [GNC20]. **template** [RS21]. **temporal** [BS20]. **tension** [BSMB23]. **tensor** [KKK23, MAMB+22]. **tensors** [JAZ+20]. **terahertz** [TLT+22]. **terbium** [GYC20]. **terbium-doped** [GYC20]. **Terminal** [MZ23, ZLG22, ZPS+20]. **Ternary** [LYW+20, CZGW22, KYL+20, WJF+21, WXHX22]. **terphenyl** [INV22b]. **terpyridine** [PS22, RR23]. **terthiophene** [SV21]. **tested** [LAAP21]. **testing** [hHRN+23]. **tetra** [LLMQ20, MM20, MSOA23]. **tetra-atomic** [MM20]. **tetra-coordinated** [MSOA23]. **tetra-N-heterocyclic** [LLMQ20]. **tetraazaacene** [FSR+22]. **tetraborate** [ZZL+20a]. **tetraborides** [SDL+23]. **tetracoordinate** [ILPY+23, TT21a]. **tetracyclic** [BDEM21]. **tetramerization** [YZD+21]. **tetramers** [Ram23]. **tetraphenyldipyranylidene** [NIA21]. **tetraphenylethylene** [PS22]. **tetrazine** [XWJ+21, ZJW+21]. **tetrazines** [HH23]. **tetrazole** [ZZXT21]. **tetrazole-based** [ZZXT21]. **tetrazolo** [ZZXT21]. **tetrel** [HLL20b, LL21]. **tetroxide** [Kid21]. **Teukolsky** [CSS+21]. **Th** [WTC+23]. **their** [BRHECY+22, Boz21, ELH20, FMS+22, KKH21, LCT+22, LYFL21, LCX+21, LPH22, MSOA23, dAOdASP+20, SMMP+23, ZLT+20]. **theorem** [Sør21]. **Theoretic** [IRA+20, OMA21]. **Theoretical** [AN20, ASHPHCB20, BBAA21, CRGD+23, CYJC20, CBK+20, DYG21, FK20, GG20b, HBB+21, KWWZ20, Kan22, KKRR21, LWW20, LXZ+21a, LG21, LZL+23, LYTS20, LL20, LLMQ20, LLQ+21, LZZ+20, MSM+20, MFC20b, MI20, PSJ22, QLGZ23, RG20, RDMF21, Roy20, SSIE21, SCZ21, SFPH22, SWML23, SWXM23, SDL+22, STT20, SYZF22, SYL+21, SYT+21,

SXTZ23, TSW+20, WLP+20, WWM+22, WWZ+20, WZL+21, WSSD21, WAW+21, WZL23, XPZ20, XHX+20, YCL+23, YYL21, ZL21, ZHD+23, ZZLY22, AAM+20, AR22, BHN23, BA21, BESG22, CCZ20, CSTD22, DYJ+22, GTAL23, HFF22, Kid21, LZS20, LK20, LCT+22, LNC+23, LYT+20, LTC+23, MZXL21, MFJ+23, MRI20, MWCJ23, MWBQ20, MK21, Mka20, MOB21, dAOdASP+20, RINHY20, Röh21, SKG23, SRS21, XZGS23, XHS+23, Yan21, YHZ+22, ZZ22, KML23, SLL+22].
theoretical-experimental [DYJ+22]. **Theoretically** [ZWL22, RKI20].
Theory [BVL22, AAYA23, AIB21, ASO+22, ABDD22, ARRB+21, BY23, BBAA21, BZP+20, BRB+21, BB20, BWBR21, BSH+21, CLW21, CXZ+21, CPL+21, DRV20, DPC+20, DFK20, EGLJQ+21, FFBH21, FMM+23, GRFM20, GMO+20, GTV20, HLL20a, ID21, Jan22, JZL+21, KZ21, KRS+21, KPMAB22, KVCS21, KYL+20, Kön21, KS23, LT23, LLW+21, LK21, sLsHtW+23, LLX+23, LCP21, LSS+21, LDS+23, MSKA20, MKKK22, MF21a, MSADA21, MAMB+22, MIM21, MB23, MP20, MHG+23, Nag20b, Nag22, NHNO20, OKK+22, PM22, PD22, Pev21, PCEAG23, QdOdMC+21, QOM+20, RBJ23, RSD21, SSEI21, Sah21, SM22, SPF+22, SAP22, SK20, STN20, SK21, SF20a, SGWW22, Shi21, SSS23, SBJ20, SG20, STF21, Sur20, Sur22, TXW+20, THL+21, TSS+23, TCX+22, TAS21, WZ20, WAM+20, XZ20, XQJ+21, XWS+22, YHW+23, YZD+21, ZZZ+20a, ZXS21, ZHG+22, ZS21].
theory [ZHS21, dPZFM+22, AMRS22, TEEH23]. **theory-based** [SK20, SSS23]. **Theory-Study** [TEEH23]. **Theory/Polarizable** [BVL22].
theory/time [WZ20]. **theory/time-dependent** [WZ20]. **there** [TLL23].
Thermal [HKM+23, TCX+22, YHZ+22, ARRB+21, BRB+21, CYL+23, CMGH+21, CMM+22, FCL22, LYPD23, LZL+23, MKKA21, MWC+21, PKBZ20, SYD+23, WWZ+20, WOE+22, YFX+22, ZZLY22]. **Thermally** [KK23a]. **thermo** [RKA+21]. **thermo-physical** [RKA+21].
Thermochemical [Iri20, Iri21, GTC+23]. **Thermodynamic** [Ram23, CP23, FWJ+23, FAB+23, FAJOF20, GNC20, JZX+20, JZL+21, KLRS22, KHK+23, KMG22, LCT+22, LMA21, MGK23, MBM+21, NR21, NLA+21, ONH+21, PL20, Pan22, PD22, WXHX22]. **thermodynamics** [YFX+22]. **thermoelectric** [AAJ+23, AAB22, AAM+20, GSRG22, GUUG23, HBB+21, KLRS22, LHZG23, MTA+22, ONH+21, RMLPGHP20, SG22, TMH21, WWLL21, tZNb+22].
thermomechanical [UV20]. **thermophysical** [SG20]. **thiahelicenes** [KM21b]. **thickness** [SAP22]. **thieno** [PGPHAPM20]. **thiobarbituric** [LYT+20]. **thiolate** [PD22]. **thione** [dLRdLJ+20]. **thionyl** [GHZ+23].
thiophene [MC22]. **thiophenol** [dLRdLJ+20]. **thiourea** [BT23]. **third** [ZQZ+23a]. **third-order** [ZQZ+23a]. **Three** [EPMC20, AMRS22, DKK+20, KMH+20, LHZG23, Xav23]. **three-centered** [DKK+20]. **three-dimensional** [KMH+20, LHZG23]. **threefold** [Tia21].
throughput [BWR22, XFW+20]. **thymine** [MHD20]. **Ti** [GGUU21, KYL+20, MHS21, CSL+23, FGW+22, KC23, RCM+22, WXHX22, XCZ+21].
Ti-modified [XCZ+21]. **TiAl** [OMA21]. **TiAl-M** [OMA21]. **Tietz**

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LCH+22, LLX+23, LCP21, MAMB+22, MB23, MSI22, NZ20, NYX+22, ORL+20b, PPCF+20, PRC23, RS23, RNH23, SBA21, STI20, SAP22, SI20, SS21, STT20, SYL+21, Tak22a, WFG+21, ZL23].

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LCY+23, SKR+21, SE22, TSS+23, ÜB20, WWM+22, WCZ+20, XBK+20]. **wave** [CPK22, Dau21, KA23, NdVVT22, NZ20, PMdN21, PS23a, STI20, Sør21, SY21, TLL23, TVdVN21, TVdVN22]. **Wavefunction** [Höf21, CFJ20, NSM22, RKI20]. **wavefunction-in-DFT** [RKI20]. **Wavelength** [Hua20]. **Wavelength-decomposition-based** [Hua20]. **wavelengths** [WKH20]. **way** [BXWK22, TLL23]. **weak** [TLT+22]. **weighted** [RNA22]. **well** [SD20]. **wells** [KRB20, Ole20, TAMU+23]. **white** [ARBM21]. **Wiener** [ADZA21, Hao21, IMJ21b, Ye20, ZZL20b]. **Wigner** [TAS21]. **wiki** [Nag20a]. **wires** [YZY+22]. **withdrawing** [FFBH21, SCAD+20]. **within** [AMM21, GOT+23, HTNP21, HRA+22, LFRTRP+20, MKD21, MB23, QDOC+21, Rac21, RPT21b, STN20]. **without** [Cio22, ZHD+23, ZHFD+20]. **WO** [JXYL20]. **women** [EPMC20]. **work** [WWM+21]. **Working** [PM22, TCL+21]. **worthwhile** [GTV20, SSEI21]. **WS** [NHH22, SIM23]. **WTe** [SCY+23]. **WX** [SPF+22].

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Anonymous:2021:IIo

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Anonymous:2021:IIp

[Ano21-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(16):e26309:1–e26309:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIq

[Ano21-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(17):e26311:1–e26311:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIr

[Ano21-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(18):e26313:1–e26313:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIs

[Ano21-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(19):e26315:1–e26315:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIt

[Ano21-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(20):e26317:1–e26317:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIu

[Ano21-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(21):e26319:1–e26319:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIv

[Ano21-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(22):e26321:1–e26321:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIw

[Ano21-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(23):e26323:1–e26323:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIx

[Ano21-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(24):e26325:1–e26325:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:ESB

[Ano22a] Anonymous. Erratum: [Simon Brezovnik and Niko Tratnik, General cut method for computing Szeged-like topological indices with applications to molecular graphs, IJQC **121**(6) 2021, e26530]. *International Journal of Quantum Chemistry*, 122(10):e26903:1–e26903:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [BT21].

Anonymous:2022:IIa

[Ano22b] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(1):e26691:1–e26691:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIb

[Ano22c] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(2):e26693:1–e26693:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIc

[Ano22d] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(3):e26695:1–e26695:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IId

[Ano22e] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(4):e26697:1–e26697:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIe

[Ano22f] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(5):e26699:1–e26699:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIf

[Ano22g] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(6):e26701:1–e26701:??, March 15,

2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIg

[Ano22h] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(7):e26703:1–e26703:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIh

[Ano22i] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(8):e26705:1–e26705:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIi

[Ano22j] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(9):e26707:1–e26707:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIj

[Ano22k] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(10):e26709:1–e26709:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIk

[Ano22l] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(11):e26711:1–e26711:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIl

[Ano22m] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(12):e26713:1–e26713:??, June 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIm

[Ano22n] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(13):e26716:1–e26716:??, July 5,

2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIn

[Ano22o] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(14):e26717:1–e26717:??, July 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIo

[Ano22p] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(15):e26719:1–e26719:??, August 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIp

[Ano22q] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(16):e26721:1–e26721:??, August 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIq

[Ano22r] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(17):e26723:1–e26723:??, September 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIr

[Ano22s] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(18):e26725:1–e26725:??, September 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIs

[Ano22t] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(19):e26727:1–e26727:??, October 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIt

[Ano22u] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(20):e26729:1–e26729:??, October

15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIu

[Ano22v] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(21):e26731:1–e26731:??, November 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIv

[Ano22w] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(22):e26733:1–e26733:??, November 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIw

[Ano22x] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(23):e27028:1–e27028:??, December 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIx

[Ano22y] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(24):e26736:1–e26736:??, December 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:E

[Ano23a] Anonymous. Erratum. *International Journal of Quantum Chemistry*, 123(8):e27080:1–e27080:??, April 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIa

[Ano23b] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(1):e26926:1–e26926:??, January 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIb

[Ano23c] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(2):e26927:1–e26927:??, January

15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIc

[Ano23d] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(3):e26928:1–e26928:??, February 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IId

[Ano23e] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(4):e26929:1–e26929:??, February 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIe

[Ano23f] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(5):e26930:1–e26930:??, March 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIf

[Ano23g] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(6):e26931:1–e26931:??, March 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIg

[Ano23h] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(7):e26932:1–e26932:??, April 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIh

[Ano23i] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(8):e26933:1–e26933:??, April 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIi

[Ano23j] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(9):e26934:1–e26934:??, May 5,

2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIj

[Ano23k] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(10):e26935:1–e26935:??, May 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIk

[Ano23l] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(11):e26936:1–e26936:??, June 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIl

[Ano23m] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(12):e26937:1–e26937:??, June 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIm

[Ano23n] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(13):e26938:1–e26938:??, July 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIn

[Ano23o] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(14):e26939:1–e26939:??, July 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIo

[Ano23p] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(15):e26940:1–e26940:??, August 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIp

[Ano23q] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(16):e26941:1–e26941:??, August

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Anonymous:2023:IIq

[Ano23r] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(17):e26942:1–e26942:??, September 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIr

[Ano23s] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(18):e26943:1–e26943:??, September 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIs

[Ano23t] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(19):e26944:1–e26944:??, October 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIt

[Ano23u] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(20):e26945:1–e26945:??, October 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIu

[Ano23v] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(21):e26946:1–e26946:??, November 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIv

[Ano23w] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(22):e26947:1–e26947:??, November 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIw

[Ano23x] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(23):e26948:1–e26948:??, Decem-

ber 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2023:IIx

[Ano23y] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 123(24):e26949:1–e26949:??, December 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arrue:2020:RAA

[APR20] Lily Arrué and Ricardo Pino-Rios. Revisiting (anti)aromaticity and chemical bond in planar B_XN_X clusters (x = 2–11). *International Journal of Quantum Chemistry*, 120(22): e26403:1–e26403:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andritsos:2022:ATS

[AR22] Eleftherios I. Andritsos and Kevin Rossi. Accelerating the theoretical study of Li-polysulfide adsorption on single-atom catalysts via machine learning approaches. *International Journal of Quantum Chemistry*, 123(8):e26956:1–e26956:??, September 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

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[ARBM21] Raúl Alvarado, Nicolás Ramos-Berdullas, and Marcos Mandado. On the adsorption affinity of graphene and white graphene sheets by dioxin-like pollutants. *International Journal of Quantum Chemistry*, 121(9):e26591:1–e26591:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

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[Ari21] Isuru R. Ariyarathna. Superatomic nature of metal encapsulated dodecahedrane: the case of $M@C_{20}H_{20}$ (M = Li, Na, Mg^+). *International Journal of Quantum Chemistry*, 121(20):e26774:1–e26774:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

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[ARRB+21] Ahmed Azzouz-Rached, Habib Rached, Majibul Haque Babu, Tariq Hadji, and Djamel Rached. Prediction of dou-

ble transition metal $(Cr_{1-x}Zr_x)_2$ AlC MAX phases as thermal barrier coatings: Insight from density functional theory. *International Journal of Quantum Chemistry*, 121(20): e26770:1–e26770:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alikhani:2022:ISB

[AS22] M. Esmail Alikhani and Bernard Silvi. Isomerism in secondary bonded complexes: Do structural rules apply? *International Journal of Quantum Chemistry*, 122(8):e26670:1–e26670:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Albrecht-Schmitt:2020:TEC

[ASHPHCB20] Thomas E. Albrecht-Schmitt, David E. Hobart, Dayan Páez-Hernández, and Cristian Celis-Barros. Theoretical examination of covalency in berkelium (IV) carbonate complexes. *International Journal of Quantum Chemistry*, 120 (15):e26254:1–e26254:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

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[ASO+22] Juan Andrés, Vicent S. Safont, Mónica Oliva, Kacee L. Caster, and Fabien Goulay. A bonding evolution theory study of the reaction between methylidyne radical, $CH(X^2\Pi)$, and cyclopentadiene, C_5H_6. *International Journal of Quantum Chemistry*, 122(11):e26892:1–e26892:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2020:IDC

[ATL+20] Diego R. Alcoba, Alicia Torre, Luis Lain, Ofelia B. Oña, Elías Ríos, and Gustavo E. Massaccesi. Incorporating dynamic correlation into the variational determination method of the second-order reduced density matrix in the doubly occupied configuration interaction space. *International Journal of Quantum Chemistry*, 120(15):e26256:1–e26256:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boda:2021:DFT

[BA21] Anil Boda and Sk. Musharaf Ali. Density functional theoretical tailoring of electronic effect through various substituents

on calix[4]arene-crown-6 for efficient Cs^+ ion encapsulation and extraction. *International Journal of Quantum Chemistry*, 121(2):e26436:1–e26436:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barp:2022:EPE

[BA22a] Marcos V. Barp and Felipe Arretche. Electron and positron elastic scattering by non-central potentials: Matrix elements and symmetry properties in the first Born approximation. *International Journal of Quantum Chemistry*, 122 (13):e26909:1–e26909:??, July 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barp:2022:YTI

[BA22b] Marcos V. Barp and Felipe Arretche. Young-type interference in soft lepton scattering of diatomic homonuclear molecules. *International Journal of Quantum Chemistry*, 122(10):e26882:1–e26882:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bahar:2022:EOR

[Bah22] Mustafa Kemal Bahar. Erratum to: Optical response of plasma processed quantum dot under the external fields. *International Journal of Quantum Chemistry*, 122(9): e26893:1–e26893:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [KB21].

Ben-Asher:2020:CAP

[BAM20] Anael Ben-Asher and Nimrod Moiseyev. Complex absorbing potentials for Stark resonances. *International Journal of Quantum Chemistry*, 120(2):e26067:1–e26067:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bouras:2020:ISM

[BB20] Farida Bouras and Ali Bentouaf. Investigation of structural and magnetoelectronic properties of new half-metallic Heusler alloys $Ru_2VGe_xSb_{1-x}$ ($x = 0$, 0.5 and 1): a density functional theory study. *International Journal of Quantum Chemistry*, 120(24):e26413:1–e26413:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

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[BBAA21] Abdelghani Benaïssa, Ali Bentouaf, Brahim Aïssa, and Boucif Abbar. Theoretical study of magneto-electronic properties of $TmCo_2$ and $NdCo_2$ intermetallic compounds through density functional theory calculations. *International Journal of Quantum Chemistry*, 121(5):e26488:1–e26488:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buzzanca:2020:ICE

[BBG20] Marissa Buzzanca, Brandon Brummeyer, and Jonathan H. Gutow. Improving convergence of experimental and computed vertical ionization energies using the ionization potential equation-of-motion coupled-cluster with singles and doubles method. *International Journal of Quantum Chemistry*, 120(18):e26261:1–e26261:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bedniakov:2023:MEC

[BBTN23] Aleksandr S. Bedniakov, Denis Bokhan, Dmitrii N. Trubnikov, and Yulia V. Novakovskaya. Modified explicitly correlated Fock-space coupled-cluster method for modeling confined molecular systems. *International Journal of Quantum Chemistry*, 123(1):e27010:1–e27010:??, January 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barysz:2021:AMR

[BCKN21] Maria Barysz, Ivan Cernusák, Vladimir Kellö, and Pavel Neogrády. AuSi molecule revisited: IOTC/CASSCF/CASPT2 calculations. *International Journal of Quantum Chemistry*, 121(5):e26502:1–e26502:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:2022:UPT

[BCLM+22] Jiang Bian, Anthony Cruz, Gabriel López-Morales, Anton Kyrylenko, Donna McGregor, and Gustavo E. López. Understanding proton transfer in non-aqueous biopolymers based on helical peptides: a quantum mechanical study. *International Journal of Quantum Chemistry*, 122(19):

e26964:1–e26964:??, October 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bako:2022:ICD

[BCM+22] Imre Bakó, Dániel Csókás, István Mayer, Szilvia Pothoczki, and László Pusztai. The influence of cations on the dipole moments of neighboring polar molecules. *International Journal of Quantum Chemistry*, 122(8):e26758:1–e26758:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

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[BCM23] Sebastian Bichelmaier, Jesús Carrete, and Georg K. H. Madsen. Evaluating the efficiency of power-series expansions as model potentials for finite-temperature atomistic calculations. *International Journal of Quantum Chemistry*, 123 (11):e27095:1–e27095:??, June 5, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balachandran:2021:EGG

[BDEM21] Selvaraj Balachandran, Hanyuan Deng, Suresh Elumalai, and Toufik Mansour. Extremal graphs on geometric-arithmetic index of tetracyclic chemical graphs. *International Journal of Quantum Chemistry*, 121(5):e26516:1–e26516:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Botella:2022:SCA

[BESG22] María Botella, Ignacio Ema, Jesús San Fabián, and Jose Manuel García de la Vega. Searching conformational analysis of Asp residues through theoretical^3 J vicinal coupling constants and Karplus equations. *International Journal of Quantum Chemistry*, 122(21):e26979:1–e26979:??, November 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bai:2022:FDP

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Biag:2022:SLE

[BGK+22] Maryam Biag, Ammal Ghaffar, Muhammad Aslam Khan, Farooq Khan, and Shanawer Niaz. Slow light effect in hybrid optomechanical system. *International Journal of Quantum Chemistry*, 122(1):e26814:1–e26814:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

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[BGM+23] Lukas Bucinsky, Marián Gall, Ján Matúska, Michal Pitonák, and Marek Steklác. Advances and critical assessment of machine learning techniques for prediction of docking scores. *International Journal of Quantum Chemistry*, 123(24):e27110:1–e27110:??, December 15, 2023. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ball:2020:EUS

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