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

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

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

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Title word cross-reference

(n, 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].
 $1s^2$ [NZA21]. 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, UB20]. 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]. ⁺
[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]. ²Π
 [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]. ⁻¹₁₁ [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]. ⁽⁻¹⁾₂
 [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, fXmTIS⁺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]. ²⁻₄ [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, OGSP⁺22, SNL⁺23, SP20b, TSS⁺23, Yan21, ZZZ20b]. *n*=1–4 [FK20]. *n*=1–4 [FK20]. *n*⁺ [ÜB20]. *n*⁻ [WYL22]. *n*^{-0/+} [TT21b]. *n*^{0/-} [DCY21]. *n*^{0/-} [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]. *ℒ_q* [SSD22, SD23]. *·* [SKR⁺21, WLLS21, WLLS21]. *···* [MOB21, SLL⁺22]. *Δ* [JXM22]. *η'* [LYPD23]. *g* [JAZ⁺20]. *γ* [SUG20, Sur20, Sur22]. *J* [OR21]. *k* [SBKT23, Zhu21, ZZL20b]. *l* [MWCJ23, PGROM20]. *λ* = 0, ±1 [LDK23]. *λ*³ [NHNO20]. *m* ≠ 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 [OGSP⁺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* ≥ 2:1 [SNL⁺23]. *n* → π* [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]. Σ3[110](111) [PP23]. *t* [CMM⁺22]. → [JWZZ20, WY20, WCZ⁺20]. *x* [APR20, BB20]. *X*²Π [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-oxethoxy** [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, WWWW21, 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** [CLW⁺22, 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]. **antietimetic** [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, ZZZ⁺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, RNFCMC20, SJ20, SMM⁺23, TAMU⁺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, AAAAAA23, 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, RDB⁺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, WXL21, WCZ⁺20]. **beyond** [GTV20]. **BH** [fXmTIS⁺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, KP21, 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 [WVZ⁺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, fXmTIS⁺23]. **Catalytic** [GOS20, AKKN20, ES21, KS23, LZL⁺21, SE20, fXmTIS⁺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, fXmTIS⁺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]. **CIO** [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, fXmTIS⁺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, RNFM20, 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 [RDB⁺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** [WXML21, 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]. **Cr mer** [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, fXmTIS⁺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,
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detecting [LZ23]. **determination** [ATL⁺20, HLL20a, PS23a, PS23b].
determining [SP20a]. **Deterministic** [BRF21]. **detonation** [LL20].
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 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**
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Differentiation [CLW21]. **diffuse** [VP20]. **diffusion**
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[Dau21, Dau23, HSV22]. **driven** [CDG⁺21, KRB20, TSN⁺21, WAM⁺20].
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Editorial [SSL22]. **education** [MNN⁺20, Shi20]. **Effect**
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effective [DFB20, KV23, KAG⁺20, MZT20, VKK⁺21, ZAB⁺23]. **effectively**
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electric-field [FAX⁺23]. **electrical** [HFF22, Rac21]. **electride**
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 [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, RNFM20, 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, KKL21, 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, QLGG23, 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, AAAAAA23, 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, fXmTIS⁺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** [LMAA21]. **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, OGSP⁺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, RNFCM20, 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,
 OGSP⁺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**
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 [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**
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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**
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TFF⁺22, TVdVN21, TVdVN22]. **fundamental** [BFW⁺22]. **fundamentals**
[CM21]. **funga** [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**
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 [Sha20]. **Gaussians** [JIFM22]. **Gd** [NG20]. **GDB17** [MJH⁺22]. **GDY**
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 [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, OGSP⁺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** [OGSP⁺22]. **HfSSe** [OGSP⁺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, RDB⁺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, fXmTIS⁺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]. **hydroxylmethyolfurfural** [LSS⁺21]. **hydroxymethyolfurfural**
 [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, RDB⁺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, OGSP⁺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, EC21, 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, AAAA23, 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** [OGSP⁺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, KPMA22, 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, KLR22, 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, fXmTIS⁺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, fXmTIS⁺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, fXmTIS⁺23]. **NHC** [LZ21]. **NHC-catalyzed** [LZ21]. **Ni** [EB22, KYL⁺20, KC23, DB20, EB22, MHG⁺23, RSD21, UBV⁺21, fXmTIS⁺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, WXL21, 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, KPMA22, 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** [RDB⁺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]. **phenylazaindoles** [HKM⁺23]. **phenylene** [CL22, FYL21, LZS20, LMAA23]. **phenylenediamines** [XZGS23]. **phenylenes** [LG22]. **phenylethylammonium** [SYZF22]. **phenylindol** [BSMI23]. **Philicity** [MB23]. **phonon** [PKBZ20]. **phores** [LYT⁺20]. **phosphide** [fXmTIS⁺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, Ung23]. **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, MSA23, 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, OGSP⁺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, DDSB20, 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**

[HZZ22, 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, RDB⁺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, RNFM20]. **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, ZYZ⁺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-tautomerism** [SBAT23]. **spin-triplet** [TVdVN22]. **spinel** [MHG⁺23, ORL⁺20a]. **spininterface** [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, fXmTIS⁺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, RNFM20, 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** [AAB20, 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]. **tetraphenyldipyranilidene** [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]. **thiahelices** [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**

[END⁺23]. **tightest** [ZMS21]. **Time** [MSKA20, AkAR⁺21, BMF20, Jan22, KVCS21, KA23, NACP21, OO21a, OO21b, PM22, RSBK20, STN20, XZ20, ZZLC20]. **Time-dependent** [MSKA20, BMF20, Jan22, KVCS21, NACP21, OO21a, OO21b, PM22, STN20, WZ20, ZZLC20]. **time-step** [KA23]. **TiO** [CXZ⁺21, HZC21, IMJ21a, NLA⁺21, RHS⁺21]. **titania** [RF23]. **titanium** [IMJ21a, IMJ21b, KS21, LSA⁺22, RK21]. **titanium-** [KS21]. **TiX** [PASS21]. **TiXSb** [RCM⁺22]. **Tl** [SBKT23]. **TM** [CZGW22, GZWL22, KC23]. **TMAI** [Pan22]. **TmCo** [BBAA21]. **TNT** [MWC⁺21]. **TNT-RDX-AI** [MWC⁺21]. **together** [Xav23]. **tool** [Gun21]. **Topological** [BUF⁺22, Hav21, KB23, KAA21, LSG21, LS21, LPH22, QSZ23, Ali20, AA23, Ano22a, AGK23, BT21, CRC21, CSGR21, FAX⁺23, Hao21, IMJ21b, INEB23, Jah20, LAAP21, MBKA21, MA23, NS22, PS22, RNB22, RDB⁺23, SUSS23, TB22, ZMS21, OGT20]. **Topology** [BVT20, MBKA21, WV20b]. **topomerization** [BZW⁺21]. **torquoselectivity** [MAMB⁺22]. **total** [HSV22]. **toughness** [LYPD23]. **toxic** [RKA⁺21, SCY⁺23]. **toxicity** [JPSC20]. **TPA** [HFF22]. **Tr** [WLLS21]. **traditional** [BXWK22]. **training** [MNN⁺20]. **trajectories** [SA20, WAM⁺20]. **trajectory** [DGA23]. **trajectory-guided** [DGA23]. **trans** [BWLZ22, RR21]. **trans-** [RR21]. **trans-1** [BWLZ22]. **transfer** [BCLM⁺22, CCZ20, CZW21, FK20, JD20, KML23, LLMQ20, MKM⁺20, Nag20a, NTND23, SCZ21, SFP22, SE22, TWT⁺21, UHK⁺22, Üng20]. **transformation** [LLMQ20, SSEI21, YZD⁺20, YCSK20]. **transformations** [ZGCF20]. **transformed** [Izs21]. **transistors** [NIA21]. **Transition** [CZJ⁺23, MMP23, ARRB⁺21, DRV20, DTAS21, FGW⁺22, GYC20, GRZ⁺21, JXM22, KM21a, LFRTRP⁺20, MKKK22, NHNO20, OAJ21, Pan20, RHS⁺21, SDS19, SDS20, SMP23b, SDL⁺23, WLY⁺20, WWKH22, XQJ⁺21, YZY⁺22, ZHS21]. **transition-matrix** [WWKH22]. **transitions** [CSK21, JWZZ20, KLK21]. **transport** [CDD23, PSJ23, SG20, SG21]. **transporting** [LZ20]. **transuranic** [ZWL22]. **trapping** [KGSD20]. **Tratnik** [Ano22a]. **treat** [PB23]. **treated** [XZGS23]. **treating** [LAAP21, SFT⁺21b]. **treatment** [AGK23, Hav21, KAA21, MA23, RPT21b]. **treatments** [GOT⁺23]. **tree** [DL21, LG22]. **tree-like** [DL21]. **trees** [ADZA21, DTW21, DAR⁺21, LYFL21]. **TrFE** [SK20]. **tri** [ELH20, SZMM22]. **tri-cations** [ELH20]. **tri-hexagonal** [SZMM22]. **triad** [CCZ20]. **triangle** [DJC21]. **triarylmethyl** [SCZ21]. **triatomic** [KRA⁺23]. **triazine** [LNC⁺23]. **triazol** [JXL⁺21]. **triazole** [XWLZ20]. **trichloride** [sLsHtW⁺23]. **tricyclic** [SWXM23]. **triel** [CLL20, WXLL21, WLLS21]. **trifluoroacetonitrile** [ZTHW23]. **trifluoromethylated** [TXW⁺20]. **trigonal** [VSKG21]. **trimers** [Ram23]. **trinitrophenyl** [QLGZ23]. **triphenylamine** [LZ20, PIA21, YLL⁺20]. **triphenylamine-based** [PIA21]. **triphenylamine-pyrimidine** [YLL⁺20]. **triphosphate** [SASA21]. **triphosphazene** [GB21, LFRTRP⁺20]. **Triple** [Tia21, MM22c]. **Triple-ring** [Tia21]. **triples** [JBPV21]. **triplet** [LYTS20, SV21, TAUM⁺23, TVdVN22].

triply [Xav23]. **trivalent** [ZWL22]. **Trolox** [dOSdASC⁺20]. **Trolox-like** [dOSdASC⁺20]. **troposphere** [WZL⁺21, WCZ⁺20]. **tropospheric** [FMG23]. **truncated** [LLC20]. **trypanothione** [RGS23]. **Tsallis** [Lom21, Ole20]. **TSH** [CMM21]. **tubular** [Tia21]. **tunability** [KSPG23]. **tunable** [LLZC20]. **Tune** [WKH20, ZL21]. **Tune-out** [WKH20]. **tuned** [SN21]. **tungsten** [AKK⁺21, JZX⁺20]. **Tuning** [HMA⁺22, NM23, TMH21]. **turn** [TSHRS⁺20]. **turn-on** [TSHRS⁺20]. **Turning** [PGÁML21]. **tutorial** [BHH20, Doh20, HHA23, MP20]. **Tutte** [CL22]. **Twenty** [Shi20]. **twisted** [QSZ23]. **twisting** [YXKJ21]. **Two** [EAPCD20, MM22c, BMF20, CZJ⁺23, DLZ⁺21, DAR⁺21, EAPCD21, FGW⁺22, GA20, GZCY22, HAA⁺23, ILPY⁺23, KYL⁺20, LXZ⁺21a, LLX⁺23, LZZW23, LZ23, Lom21, LBG20, dRNS21, Ole21, RYC⁺20, SDS19, SDS20, SAP22, SWML23, SCY⁺23, SYZF22, TSN⁺21, XQJ⁺21, dLRdLJ⁺20]. **Two-dimensional** [EAPCD20, CZJ⁺23, DLZ⁺21, EAPCD21, HAA⁺23, LLX⁺23, LZZW23, dRNS21, Ole21, RYC⁺20, SAP22, SCY⁺23, SYZF22]. **two-electron** [Lom21, SDS19, SDS20]. **two-photon** [BMF20, GA20, LXZ⁺21a, LZ23]. **two-stage** [KYL⁺20]. **Type** [GM21, BA22b, IMJ21a, KKK23, KS21, Pan22, PGPHAPM20, PGROM20, PMGR⁺21, RMeH⁺20, RR21, Sha20, UV20, UBV⁺21, XJ20, Yal23, YSZ23, ZFB⁺20]. **typical** [SBM22]. **tyrosine** [WV21].

U [AAJ⁺23, AIR⁺23, GRZ⁺21, KC23, WTC⁺23]. **U-computations** [AIR⁺23]. **Ultra** [BWR22, NdVVT22, TVdVN21, TVdVN22]. **Ultra-compact** [NdVVT22, TVdVN21, TVdVN22]. **Ultra-fast** [BWR22]. **ultrafine** [HYC⁺21]. **ultrahigh** [ZQZ⁺23a]. **Uncommonly** [OB21b, TdV21]. **Undergraduate** [EPMC20, BHH20, CM21, MNN⁺20, Nag20a, SF20b, Shi20]. **undermines** [LK20]. **understand** [TSHRS⁺20]. **Understanding** [BCLM⁺22, KZ21, SSIE21]. **undervalued** [MP20]. **Undheim** [BXWK22]. **unicyclic** [ZZL20b]. **uniform** [LXZ21b, Zhu21, ZZL20b]. **unifying** [RC20]. **unimolecular** [CMM21, SMS23]. **Unique** [LBP20]. **uniqueness** [KZ21]. **unit** [SKR⁺21]. **unitary** [GDR21, XgZX⁺22]. **units** [LZ20]. **Unlocking** [CDD23]. **unpaired** [UR23]. **unravel** [GKPK21]. **unraveling** [JRA21, LFRTRP⁺20]. **unresolved** [ID21]. **unrestricted** [GOT⁺23]. **unsaturated** [UIIP23]. **unsaturation** [KSPG23]. **Unusual** [WLLS21, LAKJ20]. **Unveiling** [CMM⁺22, HH23]. **UO** [SGWW22, SGWW22]. **updated** [XHS⁺23]. **updates** [SSK20]. **upon** [CPL⁺21, MT23]. **upper** [LYTS20]. **uranium** [Efr23, RG20]. **urea** [BT23, BVL22, ES21]. **urea-based** [BVL22]. **uril** [MZXL21, MGK23, MI20, PSJ22]. **Use** [DFB20, KPMAB22, WWF23]. **used** [CM21, Hav21, HMA⁺22, LS21]. **user** [GPP⁺21]. **user-friendly** [GPP⁺21]. **Using** [Nag20a, Tak22b, THS20, AAJ⁺23, BSMI23, BFW⁺22, BSMB23, BBG20, CMM21, CDD23, DRV20, Eti20, FH21, GZC21, GM21, HCZ20, hHNRA23, hHRN⁺23, IAI20, JPSC20, JBPV21, KSM⁺23, KV23, LLLL20,

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].

V [LLMQ20, MTA⁺22]. **vacancies** [PZGH⁺20, ZHFD⁺20]. **vacancy** [CLLC21, GG20a, HLZZ23, RSM⁺22, SPF⁺22]. **vacancy-defective** [HLZZ23]. **vacancy-ordered** [RSM⁺22]. **Vacuum** [Efr23]. **valence** [CPK22, sLLqX⁺20, LFRTRP⁺20, QOM⁺20]. **validation** [PPR21]. **value** [HTNP21, RINH20, RNH23]. **value-added** [RINH20]. **valued** [Xav23]. **values** [BMR21, BMH21, CSGR21, DTW21, FYL21, JIFM22, LGW23, ZZJ⁺23, ZHJ⁺20]. **vanadium** [KS23]. **variant** [TB22]. **variants** [SMMP⁺23]. **variation** [BMF20, NG20]. **Variational** [BXWK22, ATL⁺20, CJVF⁺23, GDR21, NdVVT22, SBA21, SS21, TVdVN21, TVdVN22, XgZX⁺22]. **variationally** [HPAM23]. **varied** [DPC⁺20]. **various** [BA21, CLS⁺22, MM21, NG20, WV20b]. **Ve** [hHRN⁺23, RNB22]. **Ve-degree** [hHRN⁺23, RNB22]. **vector** [GN20, NACP21, OO21a, OO21b]. **vegetable** [AAN⁺21]. **velocity** [BUKA21, YFX⁺22]. **velocity-dependent** [BUKA21]. **versatile** [FMG23]. **versus** [AGK23, BXWK22, DYK22, HTNP21, QdOdMC⁺21, Var21]. **vertex** [CSGR21]. **vertex-degree-based** [CSGR21]. **vertical** [BBG20, CP23, MHD20]. **vertically** [Mok21c]. **VGe** [BB20]. **via** [AAN⁺21, AR22, AD22, FFBH21, GRZ⁺21, GUUG23, HJIO21, KA21, sLLqX⁺20, LSA⁺22, MI20, SFB20, WWLL21, ZLH⁺20b]. **Viability** [KDY⁺22]. **viable** [KRK⁺21, Roy20]. **vibration** [HJIO21]. **vibrational** [BY23, Bra21, FWY⁺22, FCL22, JVK22, KHH⁺21, KHK⁺23, Kön21, LZZ⁺20, MCP⁺20, MSOA23, NR21, ORL⁺20a, RRD⁺22, WYL22, WWF23]. **Vibronic** [KLK21, KK21]. **vicinal** [BESG22]. **Vickers** [PJ20a]. **viewpoint** [DC22, LCY⁺23]. **vinyl** [BRB⁺21]. **vinylene** [LMAA23]. **vinylsilane** [ZXS20]. **Virial** [JMOW20]. **virtual** [dOSdASC⁺20]. **virus** [LS21]. **visible** [GRZ⁺21, LYW⁺20, WZ21]. **visible-light** [WZ21]. **visualization** [CSS⁺21, ZMJ⁺20]. **Visualizing** [CRKMC21]. **Viver** [Yos20]. **voltage** [YZW⁺23]. **voltages** [KM21a]. **Volume** [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]. **volumes** [PPCF⁺20]. **vs** [HMN20, YYL21].

W [OMA21, JXYL20, UBV⁺21, Yan21]. **Waals** [ISL⁺23, UP20]. **wall** [NM23]. **walled** [NM23, SMP23a]. **warming** [GHZ⁺23, TCL⁺21]. **wastewater** [ZQZ⁺23b]. **wastewaters** [SFT⁺21b]. **water** [BVL22, FGMO20, GOS20, KMK21, KBR⁺20, LC20, LAKJ20, LYW⁺20,

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].

X [ASO⁺22, AMM21, GGUU21, JWZZ20, Kid21, LYW⁺20, MZ23, NG20, PAS⁺21, PASS21, PVR20, RCM⁺22, RKA⁺21, RMeH⁺20, SPF⁺22, SGWW22, XFW⁺20, QOM⁺20, BWBR21, HP21, HLL20b, KHK⁺23, MZ23, MSOA23, RG20, RKA⁺21, SGWW22]. **X-ray** [BWBR21, HP21, MSOA23, RG20]. **Xe** [dAOdASP⁺20, AN20, MSS22].
XGaS [LYW⁺20]. **XLPE** [ZHD⁺23]. **XO** [KHK⁺23]. **XSrH** [RMeH⁺20].
XTiO [XFW⁺20]. **XY** [NG20, AMM21].

Y-junction [NS22]. **Y6** [ZZZ⁺23]. **years** [AB21, Shi20]. **YFeO** [MAHRA⁺21]. **yl** [KPTL23]. **YN** [CMGH⁺21]. **Young** [BA22b].
Young-type [BA22b]. **Ys** [CZGW22]. **Yukawa** [SSDF23].

Z [AMK⁺20, GSMT⁺20, MBM⁺21, FAB⁺23, GUUG23, KLRS22, LMM⁺22, SG22]. **Z-HFO-1234ze** [HYHW22]. **Z-Simplified** [GSMT⁺20]. **Zagreb** [DAR⁺21, RA20]. **zeolites** [DTAS21, MSCM23]. **zigzag** [DJC21]. **zigzag-edged** [DJC21]. **zinc** [AAB22, HLF23]. **zirconium** [KS21]. **zirconium-doped** [KS21]. **Zn** [GGUU21, MHS21, MEWD20, OMA21, AAJ⁺23, CLC⁺21, LYPD23, ORL⁺20a, SKG23, SBJ20, WWM⁺22, WDS⁺20]. **Zn-based** [ORL⁺20a].
ZnO [DYJ⁺22, ER22, SBJ20]. **ZnP** [CRKMC21]. **ZnP-based** [CRKMC21].
ZnPc [CRKMC21]. **ZnS** [MIM21, ZYZ⁺21b]. **zoo** [Pev21]. **Zr** [ARRB⁺21, GGUU21, KHK⁺23, XWS⁺22, YCL⁺23, YFX⁺22]. **ZrAlB** [FGW⁺22]. **ZrB** [PL20]. **ZrC** [YCL⁺22]. **zwitterionic** [HH23].

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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:CIVi</div> |
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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:CIVj</div> |
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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:CIVk</div> |
| [Ano21h] | Anonymous. Cover image, volume 121, issue 16. <i>International Journal of Quantum Chemistry</i> , 121(16):e26310:1–e26310:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:CIVm</div> |
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Anonymous:2021:CIVn

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Anonymous:2021:CIVo

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Anonymous:2021:CIVp

- [Ano21l] Anonymous. Cover image, volume 121, issue 20. *International Journal of Quantum Chemistry*, 121(20):e26318:1–e26318:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVq

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Anonymous:2021:CIVr

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Anonymous:2021:CIVs

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Anonymous:2021:CIVt

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Anonymous:2021:CIVb

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Anonymous:2021:CIVc

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Anonymous:2021:CIVd

- [Ano21s] Anonymous. Cover image, volume 121, issue 8. *International Journal of Quantum Chemistry*, 121(8):e26294:1–e26294:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVe

- [Ano21t] Anonymous. Cover image, volume 121, issue 9. *International Journal of Quantum Chemistry*, 121(9):e26296:1–e26296:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIa

- [Ano21u] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(1):e26279:1–e26279:??, January 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIb

- [Ano21v] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(2):e26281:1–e26281:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIc

- [Ano21w] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(3):e26283:1–e26283:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

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| [Ano21x] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(4):e26285:1–e26285:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIe</div> |
| [Ano21y] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(5):e26287:1–e26287:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
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| [Ano21z] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(6):e26289:1–e26289:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIg</div> |
| [Ano21-27] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(7):e26291:1–e26291:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIh</div> |
| [Ano21-28] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(8):e26293:1–e26293:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIi</div> |
| [Ano21-29] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(9):e26295:1–e26295:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIj</div> |
| [Ano21-30] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(10):e26297:1–e26297:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |

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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:III</div> |
| [Ano21-32] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(12):e26301:1–e26301:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIIm</div> |
| [Ano21-33] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(13):e26303:1–e26303:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIIn</div> |
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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIo</div> |
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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIp</div> |
| [Ano21-36] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(16):e26309:1–e26309:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIq</div> |
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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIs</div> |
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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIt</div> |
| [Ano21-40] | Anonymous. Issue information. <i>International Journal of Quantum Chemistry</i> , 121(20):e26317:1–e26317:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). |
| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIu</div> |
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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIv</div> |
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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIw</div> |
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| | <div style="border: 1px solid black; padding: 2px; text-align: center;">Anonymous:2021:IIx</div> |
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Anonymous:2022:ESB

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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

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Anonymous:2022:IIId

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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:IIIf

- [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:III

- [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:IIIm

- [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:IIIn

- [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:IIIt

- [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:IIId

- [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:IIIf

- [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:IIo

- [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:IIp

- [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:IIq

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

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

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:IIIt

- [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-

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