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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]. $1s^2$ [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]. 6 [BA21, MSS22, QOM⁺20, ÜB20]. 60
[GZWL22]. $6\pi/2\sigma$ [ZFB⁺20]. 7 [MSS22]. 8 [MSS22]. $[3 + 2]$
[MSADA21, TXW⁺20]. $[4 + 1]$ [KZ21, YYL21]. $[4 + 2]$ [LZ21, YYL21]. +
[Ari21, ABDD22, BA21, FK20, Iri21, JWZZ20, KWWZ20, MSS22, MKD21,
MM20, PCKP20, Shi21, SPR22, Wan21]. $\frac{+}{2}$ [GRLH21]. -
[HDF⁺21, THL⁺21, WWWC21]. $\frac{1}{1}$ [Cha21a, SSK20, SPR21, SPR22]. $\frac{13}{19}$
[Cha21a, GMRKCMC21, SSK20, SK21]. $\frac{19}{2+}$ [GZC21]. $\frac{2+}{2+}$
[CLC⁺21, FAJOF20, VCM⁺21, WDS⁺20]. $\frac{2+}{2+}$ / $\frac{3+}{3+}$ [RR21]. $\frac{2}{2}$ II [ASO⁺22]. $\frac{3+}{3+}$

[MAHRA⁺21, 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} [YFX⁺22]. ₁ [NYX⁺21, WAM⁺20, XPZ20]. ₁₋₈ [Kov20].
_{1-x} [ARRB⁺21, BB20, MTA⁺22, TMH21, ZYZ⁺21b]. ₁₁⁻¹ [Yan20]. ₁₂
 [GZWL22, KMG22, PL20, YFX⁺22, dPZFM⁺22]. ₁₈ [JXYL20]. ₂
 [AII21, AMK⁺20, ARRB⁺21, BBAA21, BZP⁺20, BB20, CXZ⁺21, CLLC21,
 DRV20, EGLJQ⁺21, EB22, FK20, GNC20, GSRG22, GGUU21, HNO⁺21,
 HLL20b, HYC⁺21, HZC21, IMJ21a, JZL⁺21, KDY⁺22, KWWZ20, Kan21,
 Kan22, Kov20, LLLL20, LLZC20, LYW⁺20, LHL⁺21, LWH⁺21, LZL⁺21,
 LXWZ21, LZZ⁺20, MSS20, MKM⁺20, MKD21, MZ21, MHS21, MBM⁺21,
 MAK⁺22, NLA⁺21, dRNS21, dAOdASP⁺20, ONH⁺21, OGSPP⁺22, PAS⁺21,
 Pan20, PASS21, PVR20, PZGH⁺20, PP21, QDC⁺22, QdOdMC⁺21,
 RCM⁺22, RS21, RKA⁺21, RINHY20, RHS⁺21, RNRBFC21, Roy20, SSIE20,
 SSEI21, SSIE21, SPF⁺22, SUG20, TXW⁺20, TWT⁺21, TCX⁺22, UP20,
 ÜB20, WLP⁺20, WDS⁺20, WXL⁺21, WZL⁺21, WCZ⁺20, WAW⁺21, XPZ20,
 XHX⁺20, XQJ⁺21, XWS⁺22, Yan21, Yan20, YST⁺21, YZD⁺21, YZL⁺21b,
 ZZZ⁺20a, ZCL⁺22, ZZLY22, tZNb⁺22]. ₂₀ [Ari21, JXYL20, TWT⁺21]. ₂₁
 [ELH20]. ₂⁽⁻¹⁾ [GNC20]. ₂⁺ [Dau21, MM21]. ₂²⁺ [Yan20]. _{2d} [GMRKMCMC21].
₃ [AAM⁺20, BPB⁺20, EGLJQ⁺21, JXYL20, JZL⁺21, KDY⁺22, LFRTRP⁺20,
 LZZ⁺20, MJA20, MSS20, MAHRA⁺21, MHS21, MT21, MTA⁺22, NG20,
 ORL⁺20b, PAS⁺21, Pan22, PPCF⁺20, PCKP20, PLT⁺20, QOM⁺20,
 RINHY20, RMeH⁺20, RR21, SUG20, SBG21, TWT⁺21, TCX⁺22, WDS⁺20,
 WXL⁺21, WZL⁺21, XFW⁺20, YCPW20, YZL⁺21b, YHZ⁺22, ZZZ⁺20a,
 ZFB⁺20, ZHS21]. ₃₆ [GMRKMCMC21, Tia21]. ₃⁺ [HDF⁺21, ZFB⁺20]. _{3h}
 [PCKP20]. ₄ [EB22, KHH⁺21, KMG22, KS21, MSS20, PPCF⁺20, PC22,
 RINHY20, RR21, THL⁺21, WDS⁺20, WWZ⁺21, YZL⁺21b, YCSK20]. _{4-n}
 [OGSPP⁺22]. ₄₉ [JXYL20]. ₄⁺ [WAW⁺21]. ₄⁻ [WDS⁺20]. ₄²⁻ [HOVG20b]. ₅
 [ASO⁺22, Kan21, PP21, SRS21, WWWC21, YCPW20]. _{5.5} [PZGH⁺20]. ₅₈
 [JXYL20]. ₆
 [AMK⁺20, ASO⁺22, GSRG22, RKA⁺21, WJF⁺21, YCSK20, ZCL⁺22]. _{6,7}
 [RG20]. ₆₀ [ABDD22, CCZ20, DFK20, GMO⁺20, MZ21]. ₆₀⁻ [HL20]. _{6h}
 [GMRKMCMC21]. ₇₀ [GMO⁺20]. ₈ [LWC⁺21, MZD⁺20, QOM⁺20, SRS21].
_{92-x} [MZD⁺20]. _{*m*} [PP21]. _{*n*} [AJC⁺21, FpdS21, GNC20, GZWL22, JZL⁺21,
 MOB21, OGSPP⁺22, SP20b, Yan21, ZZZ20b]. _{*n=1--4*} [FK20]. _{*n=1-4*} [FK20].
_{*n*}⁺ [ÜB20]. _{*n*}^{-/0/+} [TT21b]. _{*n*}^{0/-} [DCY21]. _{*n*}^{0/-} [DYG21, GYC20]. _{*x*}
 [APR20, Kid21, ARRB⁺21, BB20, KYL⁺20, MZD⁺20, MTA⁺22, QOM⁺20,
 TMH21, WLP⁺20, YST⁺21, ZYZ⁺21b]. _{*y*} [KYL⁺20]. _{*z*} [KYL⁺20]. _{*α*}
 [JAZ⁺20, YZL⁺21b, ZXS20]. _{*β*} [BSH⁺21, KLT21, RKG21, ZLH20a]. _{*·*}
 [SKR⁺21, WLLS21, WLLS21]. _{*···*} [MOB21]. _{*Δ*} [JXM22]. _{*g*} [JAZ⁺20]. _{*γ*}
 [SUG20, Sur20, Sur22]. _{*J*} [OR21]. _{*k*} [Zhu21, ZZL20b]. _{*l*} [PGROM20]. _{*λ*}³
 [NHNO20]. _{*L_q*} [SSD22]. _{*m*} ≠ 0 [CSS⁺21]. _{*N*} [DDSB22, LLZ⁺20, PM20,
 SF20a, TXW⁺20, DCY21, MI20, MOB21, PSJ22, TT21b]. _{*n*} = 0, 1, 2, 3, 4
 [OGSPP⁺22]. _{*n*} = 1 [JZL⁺21, ZZZ20b]. _{*n*} = 10 [DYG21]. _{*n*} = 2

[AJC⁺21, ÜB20]. $n = 30$ [GZWL22]. $n = 5$ [PSJ22]. $n = 6$ [GYC20]. ω [DPC⁺20]. π [HLL20b, LYT⁺20, LL21, OR21, PGPHPM20, SSIE21, VM20, ZIA20, ZL21]. q [Lom21, PGROM20]. $q = 1$ [MSS22]. $q = 2$ [MSS22]. σ [KSP20, LL21, VM20]. t [CMM⁺22]. \rightarrow [JWZZ20, WY20, WCZ⁺20]. x [APR20, BB20]. $X^2\Pi$ [KRS⁺21].

&K [TWT⁺21].

-5 [BRB⁺21]. **-A-D** [XPZ20]. **-acceptor** [LYT⁺20]. **-acylhydrazones** [TXW⁺20]. **-Al** [YZL⁺21b]. **-alanine** [JAZ⁺20]. **-aromatic** [JS21]. **-based** [XZ20, 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** [OR21, SSIE21, ZIA20]. **-coupling** [OR21]. **-cyclization** [YCSK20]. **-cyclodextrin** [BSH⁺21]. **-deformed** [PGROM20]. **-diketones** [RKG21]. **-directed** [WSSD21]. **-edge** [RG20]. **-enylidene-malonitrile** [BRB⁺21]. **-exponentials** [Lom21]. **-Fe** [SUG20]. **-fluorouracil** [BSH⁺21]. **-graphs** [RA20]. **-heterocyclic** [DDSB22, LLZ⁺20, PM20]. **-hole** [HLL20b, KSP20, LL21, VM20, ZL21]. **-hydroxymethylfurfural** [LSS⁺21]. **-isoxazolines** [MSADA21]. **-lactamase** [KLT21]. **-mediated** [PD22]. **-methyl** [MSM⁺20]. **-Mo** [PP21]. **-NH** [PLT⁺20]. **-nitro-1** [JXL⁺21]. **-one** [JXL⁺21]. **-oxide** [MSADA21]. **-pyrroline-** [MSADA21]. **-rich** [MZ21]. **-S** [SK21]. **-SCF** [JXM22]. **-sequestration** [QdOdMC⁺21]. **-tensors** [JAZ⁺20]. **-type** [Pan22]. **-uniform** [Zhu21, ZZL20b]. **-valence** [QOM⁺20]. **-vinylsilane** [ZXS20].

/CNT [SUG20]. **/D** [GMRKMC21]. **/DMSO** [VOK⁺20]. **/doped** [EGLJQ⁺21]. **/doped-carbon** [EGLJQ⁺21]. **/graphene** [MI20]. **/M** [LZZ⁺20]. **/NiII** [MKM⁺20]. **/organic** [NLA⁺21]. **/S** [WAM⁺20]. **/SiO** [WLP⁺20].

1-54 [RPT21a]. **1.0** [Boz21]. **12-hexaazaisowurtzitane** [ZGCF20]. **12-hexanitro-2** [ZGCF20]. **120** [Sur22]. **121** [Ano22a]. **1234ze** [HYHW22]. **15-19** [Yan21]. **19** [KAA21, LAAP21]. **1D** [CSK21, WZ21].

2 [KMK21, PPR21, Cha21b, TCL⁺21, YCSK20]. **2-** [BRB⁺21, PPR21, ZWL22]. **2-3-** [BRB⁺21]. **2-amino-2-oxyethoxy** [ZWL22]. **2-dimethylcyclohexyl** [BWLZ22]. **2'-hydroxyphenyl** [KMK21]. **2-methoxyethyl** [YST⁺21]. **2-methyl-1** [SRS21]. **2-R-C** [YCSK20]. **2D** [CRC21, LK21, RMLPGHP20, WZ21]. **2D/1D** [WZ21]. **2H** [LZ21]. **2H-azirines** [LZ21].

3 [LZS20, EM21]. **3'** [LZS20]. **3-cyclohexanedione** [MOB21]. **3-dimethylcyclohexane** [BZW⁺21]. **3-enynes** [YYL21]. **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-dithiafulvene** [ZKP22]. **4-hexadienal** [SYT⁺21]. **4-hexafluoro-** [WWZ⁺20]. **4-phenylene** [LZS20]. **4-triazol-** [JXL⁺21]. **4d** [RHS⁺21].

5-d [ZZXT21]. **5-dimethyl-** [KMK21]. **5-dimethylcyclohex-** [BRB⁺21]. **5-tetrazine** [ZJW⁺21].

7 [ZZLY22].

8 [RDMF21]. **8-hydroxyquinoline** [SFPH22].

= [AMK⁺20, Ari21, APR20, AMM21, BB20, DCY21, GGUU21, HBB⁺21, HDF⁺21, JWZZ20, Kid21, LYW⁺20, MOB21, MBM⁺21, MEWD20, NG20, dAOdASP⁺20, OMA21, PAS⁺21, PASS21, PVR20, PZGH⁺20, PCKP20, QOM⁺20, RKA⁺21, RMeH⁺20, SPF⁺22, Shi21, Tia21, TT21b, XFW⁺20, Yan21, Yan20].

A-D-A [GXL⁺22]. **ABC** [LYFL21]. **abilities** [THS20]. **Ability** [dPZFM⁺22]. **absorbing** [BAM20, JBPV21]. **absorption** [BWBR21, GA20, HSV22, HP21, INV22b, KMK21, KK21, KLK21, RG20, STI20]. **absorptive** [PAS⁺21]. **ABX** [BPB⁺20]. **Accelerating** [WV21]. **Acceleration** [GKK21]. **acceptor** [BSS21, CZW21, GXL⁺22, KMH⁺20, LFRTRP⁺20, LYT⁺20, PGPHAPM20]. **accuracy** [GZC21, KRS⁺21, ÜB20]. **Accurate** [MRI20, WWL21, ZYZ⁺22, KMK21, KAG⁺20, OB21b, TdV21, TVdVN21, TVdVN22, VKK⁺21]. **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, MBR21a, Roy20, RED21, SDL⁺22, SLdS20, WWWC21, WCZ⁺20, ZWL22]. **acid-base** [WWWC21]. **acid-based** [FFBH21]. **acidic** [LZL⁺21]. **acidity** [PVR20]. **acids** [BVT20, HYY20, LC20, MZXL21, ZLT⁺20]. **actinide** [KKH21]. **activated** [KWWZ20, NHNO20]. **activation** [dSFdSdMm20, LWR21, PPCF⁺20, STF21]. **active** [CN21, GKPK21, HP21, MWBQ20, WFG⁺21, YXKJ21]. **activities** [RHS⁺21]. **Activity** [RSD21, GOS20, YCSK20, dPZFM⁺22]. **actually** [Cio22]. **acyl** [WLH⁺20]. **acylhydrazones** [TXW⁺20]. **adamantadine**

[Bra21]. **adapted** [AIB21]. **added** [RINHY20]. **addition** [DYK22, JJJM21, LLZ+20]. **additive** [LAAP21]. **additives** [UBV+21]. **adducts** [ZPS+20]. **adenine** [MHD20]. **adenine-thymine** [MHD20]. **adenosine** [SASA21]. **adhesion** [SPF+22]. **adiabatic** [CMM21, MM21, TPB+20]. **adsorbed** [DK21]. **adsorbents** [FAJOF20].

Adsorption [HYY20, ID21, THL+21, ARBM21, CXZ+21, DJC21, JXYL20, LQZ+21, QDC+22, RBJ21, RDMF21, STI20, SBJ20, WXL+21, XCZ+21, YZL+21b]. **adsorptivity** [HLL20b]. **advanced** [MTA+22]. **advances** [PAS+21, SF20b]. **aerosols** [LRG+20]. **affinity** [ARBM21]. **Ag** [GSRG22, LYW+20]. **AgBiBr** [ZCL+22]. **agent** [HYC+21]. **aggregates** [CRKMC21]. **aggregation** [SYL+21]. **aggregation-induced** [SYL+21]. **Aharonov** [GN21b]. **AIMD** [ZKP22]. **air** [BSS21]. **Al** [MBM+21, ER22, KYL+20, LLW+21, MWC+21, RS21, TSHRS+20, YZL+21b]. **Al-doped** [ER22]. **alanine** [JAZ+20]. **AIC** [ARRB+21]. **alchemy** [GKK21]. **alcohol** [LWW20]. **alcohols** [LLLL20]. **aldehydes** [LLQ+21]. **Alder** [ABDD22]. **aldimine** [LLZ+20]. **Algebraic** [SSD22]. **algorithm** [CN21]. **alicyclic** [LPH22]. **aliphatic** [LC20]. **alkali** [FK20, HDF+21, LLLL20, MCP+20]. **alkali-** [MCP+20]. **alkaline** [LL21, MCP+20]. **alkaline-earth** [LL21]. **alkaline-earth-doped** [MCP+20]. **alkaloid** [MI20]. **alkaloids** [SSK20]. **alkanes** [SC21]. **alkenes** [LG21]. **alkenylation** [WHYL21]. **alkyl** [CLW21, CMM+22]. **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, MZD+20, PKBZ20, RCM+22, TMH21, UBV+21]. **allyl** [DYK22, LWW20]. **alpha** [MNWD20]. **alterations** [JHH+22]. **alternation** [OR21]. **aluminides** [Pan22]. **aluminum** [LLW+21, RDMF21, SK20]. **always** [LFMG20]. **Alzheimer** [ZLH20a]. **ambient** [ZWW+22]. **amide** [BSS21]. **amidine** [UAH+20]. **amine** [MSM+20]. **amino** [HYY20, LC20, MZXL21, MBR21a, PPR21, YLL+20, ZWL22]. **amino-ethyl-amino** [YLL+20]. **aminolysis** [AAN+21]. **Ammonia** [FGMO20, MSM+20, VSKG21, WCZ+20]. **ammonia-water** [WCZ+20]. **among** [MM21]. **amyloid** [ZLH20a]. **amyloid-** [ZLH20a]. **Analogies** [CRC21]. **analogous** [LPH22]. **analogue** [ABDD22]. **analogues** [PM20, ZLT+20]. **analyses** [DC22]. **Analysis** [STN20, XBK+20, AA20, BUKA21, BZW+21, BWLZ22, BRB+21, GN20, GMRKMCMC21, JD20, KAA21, LS21, LPH22, LFMG20, NS22, NHNO20, Nat22, Ole21, OMA21, PVR20, SP20a, OGT20, QDOC+21]. **Analytic** [NF20, PJ20b]. **Analytical** [Fin21, TPCSD20, AB21]. **analyze** [Gun21]. **Analyzing** [DK21, Rad21]. **anatase** [RHS+21]. **anchored** [SDL+22]. **anchoring** [MZF21]. **Angular** [SDK+21, CSS+21]. **Anharmonicity** [MM22a, LNX+21, YXKJ21]. **anhydride** [WSSD21]. **anilines** [LLQ+21]. **anion** [THL+21, WWWC21, ZZL+20a]. **anion-based** [THL+21]. **anions**

[QdOdMC⁺21]. **anisotropic** [JS21, PASS21]. **Anisotropy** [YFX⁺22, GMRKMC21]. **annealing** [TSN⁺21]. **annihilation** [STT20]. **annular** [ZZXT21]. **annulation** [LZ21, YYL21, ZZZW20]. **anode** [EGLJQ⁺21, FMH⁺22, LFX⁺21]. **ansatz** [CFJ20]. **antennas** [SFPH22]. **anthracene** [YZY⁺22]. **anti** [APR20, HRA⁺22, LG21]. **anti-Hermitian** [HRA⁺22]. **anti-Markovnikov** [LG21]. **anticancer** [PSJ22]. **antimalarial** [SK21]. **antimonene** [MZF21, THL⁺21]. **antioxidant** [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, Rui22, dOSdASC⁺20, ZMJ⁺20]. **Applications** [RKI20, AMK⁺20, Ano22a, BT21, FZL⁺20, GSRG22, HBB⁺21, KM21b, LZSA20, LCX⁺21, Rac21, RP22, TMH21, WYZZ20, ZG21]. **applied** [HMBPJ⁺20, LRG⁺20]. **apply** [AS22]. **applying** [GZC21]. **approach** [EGLJQ⁺21, EAPCD20, HTNP21, HK22, Izs21, KKH21, KYL⁺20, KAG⁺20, RSBK20, Roy20, SM22, SFT⁺21b, SS21, SG21, VL21]. **approaches** [CMM21, Kön21, SBM22]. **approximant** [BXWK22]. **Approximate** [PGROM20]. **approximation** [BA22a, GTV20, Hua20, NR21, PM22]. **approximations** [EB22, RKI20, VGSS20]. **aqueous** [KK21, KLK21, LLW⁺21, SASA21]. **aqueous-phase** [SASA21]. **arbitrary** [GM21, WP22]. **arene** [BA21]. **arene-crown-** [BA21]. **arenes** [WLH⁺20, WHYL21]. **arithmetic** [BDEM21]. **aromatic** [GMRKMC21, HRTSS⁺20, JS21, PGPHPM20, YCSK20]. **Aromaticity** [PM20, APR20, SCZ21, SCAD⁺20, Tia21, ZFB⁺20]. **arrangement** [LC20]. **arrangements** [CZ21]. **Arsenene** [MZF21, THL⁺21]. **artificial** [AkAR⁺21, WWL21]. **arylation** [WSSD21]. **aspect** [MM20]. **aspects** [BUF⁺22, GNC20, HW21b, MP20]. **Assessing** [FH21, ORL⁺20a, LCP21]. **Assessment** [Cha21b, KSP20, EB22, KRS⁺21, MK21, PVR20, TSHRS⁺20, YZD⁺20, ZYZ⁺22]. **assignment** [KMK21]. **assistant** [BHH20]. **Asymmetric** [AA20, LLQ⁺21]. **asymptotics** [SSD22]. **asynchronous** [TXW⁺20]. **atmosphere** [YZD⁺20]. **atmospheric** [CMM21, LRG⁺20, MSS20, SP20a, SRS21, SYT⁺21, ZZZ⁺20a, YST⁺21]. **atom** [CRC21, DG21, DLZ⁺21, HDF⁺21, KRK⁺21, LBG20, MF21a, SBA21, SLPS20, SPF⁺22, SPR21, ZGJ⁺20, ZHJ⁺20]. **atom-field** [CRC21]. **Atomic** [AkAR⁺21, ÉC21, Gun21, MZD⁺20, BMF20, HMBPJ⁺20, HDF⁺21, Iri20, KAUB21, Lom21, MM20, RPT21a, RPT21b, SPF⁺22, SDK⁺21, SPR22, VP20, VL21]. **atomic-scale** [UBV⁺21]. **atomisation** [LCP21]. **Atomistic** [RBJ21]. **atoms** [BPB⁺20, FK20, Fin21, GZWL22, JVK22, JXM22, MR21, MAMB⁺22, NHNO20, NZ20, RNFM20, SJ20, TT21a, WAM⁺20, WKH20, XJLH21, YÇDÖ21]. **atoms-in-molecules** [NHNO20]. **Atop** [KRB20]. **Atop-the-barrier** [KRB20]. **attractive** [GOR20]. **Augmented** [SY21, VP20]. **AuSi** [BCKN21]. **Automating** [QDOC⁺21]. **avoided** [SJ20]. **AzaBODIPY** [CCZ20]. **azirines** [LZ21]. **Azure** [KLK21].

B [MZD⁺20, MBM⁺21, NG20, YFX⁺22, PGPHPM20, APR20, CPL⁺21, ÉC21, SSIE20, SSIE21, ZFB⁺20, dPZFM⁺22]. **B/N** [SSIE20]. **Ba** [Shi21, Tia21, XFW⁺20, VCM⁺21]. **backbone** [LFRTRP⁺20, ZZ22]. **Backflow** [NZ20]. **balance** [XWLZ20]. **band** [MBKA21, RK21, WWLL21, WLY⁺20]. **Bandgaps** [HZC21]. **bands** [KMK21]. **barrier** [ARRB⁺21, KRB20]. **barriers** [VKK⁺21]. **base** [GG20b, MHD20, VOK⁺20, WWWC21]. **base-promoted** [VOK⁺20]. **Based** [ZJW⁺21, AkAR⁺21, BVL22, BSS21, CN21, CRKMC21, CSGR21, DSNZ⁺20, FFBH21, FZL⁺20, GNC20, GMO⁺20, GPP⁺21, HLL20a, HRTSS⁺20, Hua20, JBPV21, JZL⁺21, JXL⁺21, JD20, KMH⁺20, KJA⁺21, KI20, KS21, LYT⁺20, LZ20, LAAP21, MSKA20, MIM21, MJRS20, NG20, dRNS21, ORL⁺20a, PIA21, RRD⁺22, RNA22, RNB22, RSD21, SIA20, SK20, SMJ20, STN20, SG20, SG21, STF21, TSN⁺21, THL⁺21, TCX⁺22, WWL21, WZ20, WJL⁺21, XPZ20, XZ20, XWJ⁺21, ZZXT21, ZZ22, ZMS21, TCL⁺21]. **bases** [RKG21, SE20]. **basic** [HW21b, LZL⁺21]. **Basis** [QdOdMC⁺21, DK21, GSMT⁺20, HMBPJ⁺20, RPT21a, STI20, SM22, SK21, SS21, VP20, Var21]. **BaTiO** [ORL⁺20b, WXL⁺21]. **batteries** [EGLJQ⁺21, MZF21, MHS21, dRNS21, ZYZ⁺22]. **battery** [FMH⁺22, LFX⁺21]. **BC** [MJA20, XHX⁺20]. **Be** [PCKP20, FGMO20, LL21, KDY⁺22, LWC⁺21]. **bearing** [LLMQ20]. **behavior** [JSF⁺21, MWC⁺21, SG21]. **being** [KAA21]. **Benchmark** [KLT21, KAG⁺20, SK21, VKK⁺21, TTTH20]. **Benchmarking** [Cha21a, JS21, PPCF⁺20, GZC21]. **benchmarks** [AIB21]. **benzamides** [ZZZW20]. **benzene** [Mok21b, RNA22, RNB22, UP20, YXKJ21]. **benzenoid** [LCX⁺21, WYZZ20]. **benzoselenadiazole-pyrrole** [SCU21]. **benzothiadiazole** [SCU21]. **benzothiadiazole/benzoselenadiazole** [SCU21]. **benzothiadiazole/benzoselenadiazole-pyrrole** [SCU21]. **benzothiazole** [PPR21]. **benzoxazinone** [SSEI21]. **benzoxazole** [LLZ⁺20]. **berberine** [KK21]. **berkelium** [ASHPHCB20]. **Bethe** [CFJ20]. **between** [ASO⁺22, CRC21, HLL20b, ID21, KZ21, KMK21, Kid21, MNN⁺20, MWBQ20, Rad21, WXML21, WCZ⁺20]. **beyond** [GTV20]. **Bi** [MAHRA⁺21]. **bicyclic** [MSADA21]. **bilayer** [CPL⁺21, Mok21c]. **binary** [Yan21]. **Binding** [MZXL21, MFC20a, CZ21, GRFM20, JXM22]. **binuclear** [DTAS21]. **BiOBr** [GRZ⁺21]. **biphenyl** [BMH21]. **bipyramidal** [VSKG21]. **bis** [BSS21, LZS20, XWLZ20, XWJ⁺21]. **bis-amide-based** [BSS21]. **bismuthene** [MZF21]. **black** [GG20a]. **block** [CL21]. **blue** [LYTS20, WLY⁺20, ZHFD⁺20]. **BN** [Roy20]. **bodipy** [TPT20, MRI20]. **body** [Eti20, LBG20, RKI20, SMJ20, UP20]. **Bohm** [GN21b]. **Bohr** [JVK22]. **boiling** [HYHW22, LCX⁺21]. **Boltzmann** [BRF21, VL21]. **Bond** [YXKJ21, AN20, AAN⁺21, APR20, CPK22, HLL20b, JD20, KLT21, KAG⁺20, LAKJ20, LNX⁺21, LL21, LAAP21, ÖCÖ21, RR21, SK20, STF21, TTTH20, WLLS21, ZZF22]. **bonded** [AS22, MOB21]. **bonding** [ASO⁺22, CSY⁺21, DKK⁺20, KSP20, Kov20, LFRTRP⁺20, NSM22, PCKP20, RNRBFC21, SFB20, VCM⁺21, ZWL22]. **bonds**

[CLL20, LL21, PC22, SI20, VM20, WXML21, ZL21]. **Book** [BRB⁺21, EM21, YST⁺21]. **boosts** [ZXS20]. **borane** [MSM⁺20]. **Born** [BA22a]. **boron** [CPL⁺21, MCP⁺20, SZMM22, THS20]. **boroxol** [ZFB⁺20]. **boroxol-type** [ZFB⁺20]. **Bose** [PMdN21]. **both** [QDC⁺22]. **bottom** [LC20]. **bottom-up** [LC20]. **bound** [PGROM20]. **boundary** [LLC20]. **Bounds** [RA20, CDR20, RMWF20]. **Box** [GSMT⁺20]. **Br** [AMK⁺20, AMM21, GSRG22, PAS⁺21, RKA⁺21]. **Braun** [CBK⁺20]. **Braun-like** [CBK⁺20]. **BrCl** [WAW⁺21]. **Brezovnik** [Ano22a]. **bridge** [CZW21]. **bridge-state** [CZW21]. **bridged** [SSIE21, XWLZ20]. **bridges** [LYT⁺20]. **bridging** [JHH⁺22]. **bright** [DSNZ⁺20]. **broadening** [UP20]. **bromanes** [NHNO20]. **bromochloroethane** [WAW⁺21]. **Building** [MNN⁺20]. **bulk** [LHL⁺21, MHD20, RC20, Yan20]. **butadiene** [BTS⁺21, SRS21]. **butene** [WWZ⁺20, YHW⁺22]. **butyl** [CMM⁺22]. **BX** [PVR20]. **Bypassing** [JJJM21].

C [Ari21, EB22, GMRKMC21, LWH⁺21, LZZ⁺20, SK21, SRS21, TWT⁺21, ASO⁺22, ABDD22, Cha21a, CCZ20, DFK20, ÉC21, GMO⁺20, GMRKMC21, HL20, JSF⁺21, KAG⁺20, LWC⁺21, LWR21, MZ21, MOB21, NZ20, RS21, RINHY20, SSK20, STF21, WSSD21, WWKH22, WHYL21, WAW⁺21, YCPW20, YCSK20]. **C-H** [WHYL21]. **C-Mg** [KAG⁺20]. **C-NMR** [GMRKMC21]. **C40** [Pan20]. **Ca** [PZGH⁺20, Tia21, XFW⁺20, WY20]. **CaCl** [WY20]. **cadmium** [FCL22]. **CaF** [HNO⁺21]. **caffeine** [KVCS21]. **cage** [AJC⁺21, ELH20, GMO⁺20, 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, STT20, TCX⁺22, WP22, XJLH21, ZS21]. **Calculations** [Cha21a, GRFM20, BCKN21, BBAA21, BVL22, CN21, CRKMC21, CXZ⁺21, GMO⁺20, GRZ⁺21, HK22, HMN20, HCZ20, JXM22, Kan22, LRG⁺20, LWH⁺21, MKD21, MP20, OGT20, OAJ21, ORL⁺20b, PL20, QdOdMC⁺21, QOM⁺20, Rac21, SBA21, SK21, THS20, WZ20, Wan21, XFW⁺20, ZRR⁺21, ZGJ⁺20, ZYZ⁺21b, ZLH⁺20b]. **calculus** [TVdVN21, TVdVN22]. **Calibration** [GKPK21]. **calix** [BA21]. **Can** [FGMO20, KM21a, LL21]. **cancer** [Hav21]. **canonic** [SM22]. **Canonical** [Var21]. **capacitance** [CLLC21, SUG20, XWS⁺22]. **capacity** [LFX⁺21, MNN⁺20]. **capped** [JHH⁺22]. **capture** [DRV20, Kan21, Kan22]. **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, LQZ⁺21, NS22, PNC20, THS20, TT21a, ZMS21]. **carbonate** [ASHPCB20, ZLH⁺20b]. **carbonated** [UV20]. **carbonates** [LLLL20]. **Carbonyl** [KBR⁺20, LZL⁺21, MSM⁺20]. **carboxylate** [LLW⁺21].

care [RBSW21b]. **career** [SF20b]. **Carlo** [HZC21, NZ20, SRH20, SS21].
carrier [Dau21, WWL21]. **carrier-envelope** [Dau21]. **Case**
 [HMN20, Ari21, INV22b, MM20, NHNO20, YCSK20]. **cases** [RRSF22].
CASPT2 [BCKN21]. **CASSCF** [BCKN21, CN21]. **catalysis**
 [HYY20, PGÁML21, SRH20]. **catalyst**
 [AKKN20, GKK21, LK21, Roy20, SDL⁺22, VKS21, WLP⁺20]. **catalysts**
 [DLZ⁺21, GKPK21, KS21, LZL⁺21, RSD21]. **Catalytic**
 [GOS20, AKKN20, ES21, LZL⁺21, SE20]. **catalyzed**
 [CYJC20, CSY⁺21, JRA21, LLZ⁺20, LZ21, LG21, LWR21, SLdS20, TXW⁺20,
 WWZ⁺21, WSSD21, WLH⁺20, YZD⁺21, YYL21, ZZZW20, CMM⁺22].
caterpillars [Ye20]. **cathode** [KM21a, MHS21]. **cation**
 [DTAS21, Iri21, MKD21, Mka20]. **cationic** [DTAS21]. **cations**
 [BCM⁺22, CYJC20, ELH20, KKH21, PCKP20]. **cavity** [BUF⁺22, YÇDÖ21].
cavity-induced [BUF⁺22]. **CC2** [JS21, JS21]. **CC3** [JS21]. **CCSD**
 [JS21, JS21]. **Celebrating** [KKRR21]. **cell** [MSKA20]. **cells** [BSS21,
 FFBH21, FZL⁺20, KMH⁺20, KJA⁺21, LZ20, PIA21, PGPHAPM20, SIA20].
Center [GM21]. **centered** [DKK⁺20, SF20a]. **centers** [SCAD⁺20]. **central**
 [BA22a, Nat22]. **cephalosporins** [KLT21]. **ceramics** [PL20, XFW⁺20].
cerium [sLhZX⁺22]. **certain** [LAAP21, RRSF22]. **CF**
 [CLLC21, LZL⁺21, TCX⁺22, YZL⁺21b, YHZ⁺22]. **CF3** [HMN20]. **CH**
 [HMN20, ZHS21, ASO⁺22, BZP⁺20, WWZ⁺21, ZZZ⁺20a, ZHS21]. **Chain**
 [DYK22, AII21, CLC⁺21, LC20, LSG21, MAK⁺22]. **chain-initiation**
 [CLC⁺21]. **chains** [BMR21, FYL21, ZZXT21]. **chalcogen** [CLL20, ZLT⁺20].
chalcogenides [LYW⁺20]. **Challenges** [SC21, GG22, ZG21]. **change**
 [RNRBFC21]. **channel** [TSHRS⁺20]. **character** [GMRKMCMC21, JJJM21].
Characteristic [CRKMC21]. **characteristics**
 [CXZ⁺21, LFRTRP⁺20, SFB20, XHX⁺20]. **Characterization**
 [JD20, AKK⁺21, RPAA22]. **Charge**
 [KVCS21, ABS20, BZW⁺20, BS20, FK20, Gun21, MKM⁺20, Mok21c, RR21,
 SCZ21, Üng20, VL21, XAM⁺22, YCPW20]. **charged** [KKH21]. **CHCl**
 [HMN20]. **Chem** [GM21, Sur22]. **Chemical**
 [Cha21a, RMWF20, WFG⁺21, 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,
 MJA20, NSM22, PCKP20, RRS21, RNB22, SM22, SBM22, SK21, Sta21,
 VKS21, VOK⁺20, ZG21, ZZF22]. **chemicals** [GG20b]. **chemist** [RBSW21b].
Chemistry
 [KKRR21, BHH20, Cio22, EPMC20, HHG⁺21, KBR⁺20, KS22, MFK22,
 MJRS20, Mos21, PGÁML21, RP22, Sha20, Shi20, VN21, WWL21, HHG⁺21].
chemodivergent [ZZZW20]. **chemosensor** [HRTSS⁺20, TSHRS⁺20].
Chirality [XAM⁺22, LNX⁺21]. **Chirality-helicity** [XAM⁺22]. **chloride**
 [DYK22]. **chlorine** [SRS21]. **chlorophylls** [SIA21]. **CHO** [ZHS21].
chromophores [GA20, SFB20]. **CHZ** [WDS⁺20]. **cigar** [PMdN21].
cigar-shaped [PMdN21]. **circular** [RG20]. **cis** [WWZ⁺20, Mka20]. **cis-1**

[WWZ⁺20]. **Cisplatin** [ZYZ⁺21a]. **Cl**
 [AMK⁺20, AMM21, PAS⁺21, PVR20, RKA⁺21, GNC20]. **Clar** [RRD⁺22].
Clar-structure-based [RRD⁺22]. **class** [LPH22, PMGR⁺21]. **Classical**
 [RRSF22, BM21, DG21]. **classically** [FGMO20]. **cleavage** [KAG⁺20]. **CIO**
 [WDS⁺20, WDS⁺20]. **cloud** [RBSW21b]. **cluster**
 [AIB21, BBG20, Cha21b, FK20, GDR21, Gun21, HTNP21, Hua20, JBPV21,
 KBR⁺20, Roy20, Var21, ZFB⁺20, ZG21]. **clusters** [AJC⁺21, APR20,
 BTS⁺21, DCY21, GNC20, GYC20, JZL⁺21, KYL⁺20, LAKJ20, MFC20a,
 MOB21, NLA⁺21, PPCF⁺20, SBJ20, TT21b, ÜB20, Yan21, ZZZ20b]. **Cmcm**
 [PP21]. **Cmcm-Mo** [PP21]. **CN** [PVR20]. **CNT** [SUG20]. **CO** [KWWZ20,
 LLZC20, XWS⁺22, DRV20, DK21, ER22, HLL20b, Kan21, LLLL20, LXWZ21,
 QdOdMC⁺21, RINHY20, SSIE20, SSEI21, SSIE21, LQZ⁺21, MZD⁺20].
coatings [ARRB⁺21]. **cobalt** [SG21, SP20b]. **cobalt-based** [SG21].
coefficient [KRS⁺21]. **coefficients** [HYHW22]. **CoF** [SP20b]. **CoI**
 [MKM⁺20]. **coindices** [DAR⁺21]. **Collaboration** [GOR20, MNN⁺20].
collision [CLS⁺22]. **combined** [GNC20, NF20, STI20, YHZ⁺22, ZKP22].
Combining [dOSdASC⁺20]. **coming** [RPT21b]. **Comment**
 [Cin20, MMM20, MAK⁺22, NACP21, TdV21, OB21a, OO21b]. **Compact**
 [WP22, TVdVN21, TVdVN22]. **Comparative**
 [JWZZ20, Ole21, AB21, HTNP21, NS22, dLRdLJ⁺20]. **Comparison**
 [CLL20, AIB21, GSMT⁺20]. **Competition** [WCZ⁺20]. **complete**
 [HP21, Var21]. **complete-basis-set** [Var21]. **completeness** [Sha20].
Complex [BAM20, UBW⁺22, JBPV21, KDY⁺22, Kön21]. **complexes**
 [ASPHCB20, AS22, CYJC20, DSNZ⁺20, EB22, Kov20, LLW⁺21, LLMQ20,
 dAOdASP⁺20, PPR21, PLT⁺20, RR21, RKG21, SFPH22, SP20a, Shi21,
 SN21, VGSS20, VSKG21, WXLL21]. **complexity**
 [EAPCD20, EAPCD21, GN21b, Nat22, SSD22]. **complexity-like** [SSD22].
compliance [MM22a]. **component** [AMM21]. **composite**
 [HYC⁺21, SBA21, SUG20, VKK⁺21]. **composites** [EGLJQ⁺21, KAUB21].
compound [HNO⁺21, sLLqX⁺20, LHL⁺21, ONH⁺21]. **compounds** [AN20,
 AMK⁺20, BRHECY⁺22, BBAA21, HBB⁺21, HRTSS⁺20, LAAP21, MSM⁺20,
 MBM⁺21, SK21, dOSdASC⁺20, SG21, XWLZ20, XWJ⁺21, Yan20, ZRR⁺21].
comprehensive [Eti20, RCM⁺22]. **compressed** [SBA21]. **comprising**
 [PC22]. **Computation** [AIAG21, CDG⁺21, MSA22, TCSG⁺20, Boz21].
Computation-driven [CDG⁺21]. **Computational**
 [AAN⁺21, ABDD22, BZW⁺21, GMRKMCMC21, JHH⁺22, KI20, KKRR21,
 LWR21, RYC⁺20, SBG21, VSKG21, WJL⁺21, ZJW⁺21, ZZZW20, BHH20,
 BSS21, BRB⁺21, CMM⁺22, EPMC20, GKPK21, GKK21, GG22, KBR⁺20,
 MZF21, MNN⁺20, ÖÇÖ21, RCM⁺22, RBSW21b, Shi20, Shi21, SCU21,
 TCSG⁺20, UBV⁺21, WLH⁺20, WHYL21]. **Computationally** [JRA21].
computed [BBG20]. **Computing**
 [NS22, Ano22a, AKP22, BT21, LSG21, RBSW21b]. **concentration**
 [CMGH⁺21, WWLL21]. **concept** [SSIE20]. **concerted** [TXW⁺20, WAW⁺21].
condensates [PMdN21]. **condensed** [RKI20]. **condensed-phase** [RKI20].

conditions [Sør21, ZWW⁺22]. **conductance** [BMH21]. **conductivity** [UBW⁺22, YFX⁺22]. **configuration** [ATL⁺20, BZW⁺20, dSFdSdMdM20, MKD21, SPR21, SPR22, ZGJ⁺20, ZS21, dLRdLJ⁺20]. **configuration-interaction** [ZGJ⁺20]. **configured** [ZMS21]. **confined** [EAPCD20, EAPCD21, LBG20, MR21, SJ20, SLPS20, YÇDÖ21, ZHJ⁺20]. **confinement** [RNFMC20, RNRBFC21]. **conformation** [WV21]. **conformational** [BZW⁺21, BWLZ22, HYY20, MBR21a, ZGCF20]. **conformer** [FH21]. **conical** [WAM⁺20]. **conjugate** [KRB20]. **Conjugated** [KOB20, KZ21, LYT⁺20, OR21, SSIE21, ZIA20]. **Conjugated-carbon** [KOB20]. **conjugation** [ZZ22]. **connective** [WYZZ20]. **connectivity** [GW21]. **consistent** [HK22, HP21, SM22, VGSS20]. **consortium** [MNN⁺20, Shi20]. **constant** [LHL⁺21]. **constants** [HYHW22, JAZ⁺20, MM22a, OAJ21]. **construct** [LWR21]. **Constructing** [TPB⁺20]. **contact** [VdM22]. **contained** [Eti20, LXZ⁺21a]. **containing** [AN20, HYC⁺21, SSEI21, TTTH20]. **content** [GZWL22]. **continuation** [LBP20]. **Continuum** [BVL22]. **contracted** [HRA⁺22]. **Control** [LNX⁺21, DSNZ⁺20]. **Controlling** [Dau21, GZCY22]. **convergence** [BBG20]. **conversion** [BTS⁺21, Kan21, LLZ⁺20, RINH20, SIA21]. **Conversions** [TWT⁺21]. **Cooperative** [WXLL21, ZL21]. **cooperativity** [MOB21, LL21]. **coordinates** [Bra21, MM22a]. **coordination** [SCAD⁺20]. **coplanar** [WJL⁺21, XWJ⁺21]. **copolymers** [BSS21, SCU21]. **copper** [SDK⁺21, ZPS⁺20]. **core** [JHH⁺22, JXM22, KMH⁺20, LNE⁺20, MZT20]. **core-level** [LNE⁺20]. **corona** [LS21]. **coronoid** [CSGR21]. **correct** [CN21]. **corrected** [EB22, GMO⁺20]. **Correcting** [CM21]. **correction** [BSH⁺21]. **corrections** [AMM21, Iri20, Iri21, XJLH21]. **correlated** [CPK22, JIFM22, SPR21, SPR22, Var21]. **correlation** [ATL⁺20, Hua20, PT21, SP20b, STT20, VP20, ZIA20, ZS21]. **correlation-polarization** [STT20]. **Corrigendum** [Ano21a, GM21, SDS20]. **corrolazine** [WWZ⁺21]. **corrosion** [UBV⁺21]. **CoSi** [ONH⁺21]. **cost** [KAG⁺20, TCSG⁺20, VKK⁺21]. **cost-effective** [KAG⁺20]. **Coulomb** [Dau21, MF21a, WWKH22, XJLH21]. **counting** [Pev21]. **coupled** [AIB21, BBG20, GDR21, HTNP21, JBPV21, Roy20, SY21, Var21]. **coupled-cluster** [AIB21, BBG20, HTNP21]. **couplers** [KA21]. **coupling** [AAM⁺20, JAZ⁺20, KWWZ20, LLLL20, MKD21, OR21, 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]. **COVID-19** [KAA21, LAAP21]. **CoZr** [TMH21]. **Cr** [ARRB⁺21, LLMQ20, YZD⁺21]. **Cr/PNP** [YZD⁺21].

Cr/PNP-catalyzed [YZD⁺21]. **Crámer** [EAPCD21]. **criteria** [Pev21].
Critical [SDS19, SDK⁺21, SDS20]. **cross** [KMH⁺20, MW21]. **crossing**
 [KWWZ20, LYTS20, SV21, SJ20, TPB⁺20]. **crossover** [KGSD20].
crotonaldehyde [CMM21]. **crown** [BA21, TT21a]. **CrSi** [Pan20]. **crude**
 [BXWK22]. **crystal** [BRB⁺21]. **crystallization** [TAS21]. **crystallography**
 [MM22c]. **Cs** [BA21, ZCL⁺22]. **CsTmCl** [AAM⁺20]. **CTDE** [YZD⁺20]. **Cu**
 [LYW⁺20, MHS21, OMA21, Yan20, BWBR21, DB20, GZWL22, SBJ20,
 TXW⁺20]. **Cu-porphyrazines** [BWBR21]. **CUAGAU** [Cha21b].
CUAGAU-2 [Cha21b]. **Cuban** [GG22]. **cubic** [ACM20, XFW⁺20].
cuboidal [PPCF⁺20]. **cucurbit** [MZXL21, MI20, PSJ22]. **cumene**
 [CLC⁺21]. **cumulenes** [XAM⁺22]. **current** [PM20, SIA21]. **Curtius**
 [LFMG20]. **curve** [Kid21]. **cusp** [Cio22, JIFM22]. **cut** [Ano22a, BT21].
cyanic [ZLT⁺20]. **cyanobenzene** [KJA⁺21]. **cyclic** [LFRTRP⁺20, Rad21].
cyclic-triphosphazene [LFRTRP⁺20]. **cyclization** [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]. **cyclooctatetraene** [CMY22].
cyclopentadiene [ASO⁺22, PVR20]. **cyclopentano** [MI20].
cyclopentano-cucurbit [MI20]. **cyclopropanol** [LWR21].

D [GXL⁺22, GMRKMC21, JWZZ20, JS21, Mka20, XPZ20, ZZXT21,
 DKK⁺20, GRLH21, GMRKMC21, JHH⁺22, MKKA21, PGPHAPM20,
 PCKP20, XPZ20]. **D-A** [JHH⁺22]. **D8** [PP21]. **dark** [DSNZ⁺20]. **Data**
 [OGT20]. **database** [TTTH20]. **DCCnT** [XZ20]. **DEAL** [KKRR21].
deamination [UAH⁺20]. **Debye** [WWKH22]. **decay** [SV21, TSHRS⁺20].
decomposition [AIB21, BWLZ22, CMM⁺22, HCZ20, Hua20, MWC⁺21,
 SDL⁺22, TCX⁺22, WWZ⁺20, YHZ⁺22]. **decorated** [MJA20, RS21].
decoration [QDC⁺22]. **Deep** [LACP21]. **deeper** [ZYZ⁺21a]. **defect**
 [CLLC21]. **defected** [AKKN20]. **defective** [LK21]. **defects**
 [QDC⁺22, RMM⁺22, SPF⁺22]. **deficient** [LZ20]. **defined** [RKI20].
definitions [CPK22]. **deformation** [AA20, MNWD20]. **Deformations**
 [BRHECY⁺22]. **deformed** [PGROM20]. **degeneracies** [BUF⁺22].
degradation [CXZ⁺21, SRS21, SYT⁺21]. **Degree**
 [SSD22, CSGR21, RNA22, RNB22, RMWF20, SF20b, Wan21]. **degree-based**
 [RNA22]. **dehydrogenation** [DB20]. **delayed** [SYL⁺21]. **delimited**
 [BVT20]. **delivery** [PSJ22]. **delocalization** [Rad21]. **dendrimers** [MSA22].
Deng [NR21]. **dense** [CLS⁺22]. **densities** [LBG20]. **Density**
 [BA21, CXZ⁺21, DRV20, DPC⁺20, KRS⁺21, MR21, SPF⁺22, Shi21, SBJ20,
 VGSS20, XWS⁺22, dPZFM⁺22, ATL⁺20, AA20, ABDD22, ARRB⁺21,
 BBAA21, BZP⁺20, BMH21, BRB⁺21, BB20, Boz21, BSH⁺21, CPL⁺21,
 Cio22, DFK20, DS20, EGLJQ⁺21, EB22, Eti20, FFBH21, GMO⁺20, GTV20,
 HMBPJ⁺20, Höf21, HW21a, Hua20, JMOW20, JZL⁺21, KZ21, KVCS21,
 KYL⁺20, KAG⁺20, KH20, LLW⁺21, LK21, LCP21, LSS⁺21, LFMG20,

MSKA20, MKKK22, MZ21, MSADA21, MIM21, MOB21, MP20, Nag20b, Nag22, OAJ21, PM22, PJ20b, Pev21, QdOdMC⁺²¹, QOM⁺²⁰, RSD21, RPT21b, SK20, SMJ20, STN20, SK21, SF20a, SG20, STF21, TXW⁺²⁰, THL⁺²¹, TCX⁺²², TT21b, WZ20, XAM⁺²², XZ20, XWLZ20, XQJ⁺²¹, YZD⁺²¹, ZJW⁺²¹, ZZZ^{+20a}, ZZLC20, ZXS21, ZYZ⁺²², ZZXT21, BVL22, PD22, SSEI21]. **density-density** [DS20]. **density-fitted** [Boz21]. **density-functional** [STN20, SF20a]. **density-to-potential** [KH20]. **dependence** [BS20, BWLZ22, CLL20, ORL^{+20b}, ZGJ⁺²⁰]. **dependent** [BUKA21, BMF20, Dau21, HW21b, HYHW22, KVCS21, sLhZX⁺²², LHL⁺²¹, MSKA20, MBKA21, NACP21, OO21a, OO21b, PM22, STN20, UBW⁺²², WZ20, XZ20, ZZLC20]. **dephasing** [CZW21]. **deposition** [LQZ⁺²¹]. **depth** [YHW⁺²²]. **Depurated** [Cin20, MMM16, MMM20]. **derivation** [Eti20]. **derivative** [HTNP21, LYT⁺²⁰, LZ20, TPT20, ZWW⁺²², dPZFM⁺²²]. **derivative-based** [LYT⁺²⁰, LZ20]. **derivatives** [Boz21, FSR⁺²², GXL⁺²², JXL⁺²¹, LL20, LPH22, MZ21, NF20, NIA21, RNA22, RNB22, SSEI21, SFPH22, SBM22, SRS21, UAH⁺²⁰, WXL21, ZJW⁺²¹]. **derived** [Bra21, XAM⁺²²]. **described** [FGMO20]. **descriptors** [Hao21, IMJ21b, JPSC20, RSD21, RC20, SZMM22, WWL21, WWLL21]. **Design** [PVR20, FZL⁺²⁰, FAJOF20, JXL⁺²¹, MFK22, SUG20, VN21, WJL⁺²¹, XWLZ20, ZZXT21]. **designed** [TSN⁺²¹]. **Designing** [KMH⁺²⁰, KJA⁺²¹, XZ20, SSIE21, SCU21]. **desorption** [FK20]. **detachment** [TSN⁺²¹]. **Detailed** [UBV⁺²¹]. **details** [MP20]. **determination** [ATL⁺²⁰, HLL20a]. **determining** [SP20a]. **Deterministic** [BRF21]. **detonation** [LL20]. **deuterium** [STI20]. **Development** [CLS⁺²², Cha21b, dOSdASC⁺²⁰]. **device** [KM21b]. **devices** [KHH⁺²¹, MTA⁺²²]. **devil** [MP20]. **DFT** [CRKMC21, CMM21, Cha21a, Cha21b, GZC21, GNC20, GRZ⁺²¹, HMN20, KLK21, LLLL20, LZ21, MKKA21, Mka20, MT21, PGPHAPM20, PVR20, PPCF⁺²⁰, Rac21, RKI20, SKR⁺²¹, XZ20, ZKP22, ZZZ20b]. **DFT-in-DFT** [RKI20]. **DFT/GIAO** [GZC21]. **DFT/periodic** [PGPHAPM20]. **DFTB** [NLA⁺²¹]. **DH** [TCSG⁺²⁰]. **DH-SVPD** [TCSG⁺²⁰]. **di-superatomic** [Yan21]. **diabatic** [MKD21]. **diagonal** [Cio22]. **diamide** [RED21]. **diamond** [HW21a]. **diamondoid** [STF21]. **diarylethenes** [NYX⁺²¹]. **diatomic** [AB21, BA22b, HSV22, HTNP21, XJ20]. **diborane** [DKK⁺²⁰]. **dichroism** [RG20]. **dielectric** [BPB⁺²⁰, HYHW22]. **Diels** [ABDD22]. **difference** [VL21]. **different** [CLL20, GZC21, GZCY22, JZX⁺²⁰, NLA⁺²¹, Rad21, RR21, Üng20, VL21, WZ21, XZ20, ZZ22]. **Differentiation** [CLW21]. **diffuse** [VP20]. **diffusion** [HYHW22, HZC21]. **difluoro** [CMM21]. **difunctionalization** [AAN⁺²¹]. **dihalogen** [AMM21]. **diiodocyclododecanes** [MF21b]. **diketone** [LWR21]. **diketones** [RKG21]. **dimensional** [DLZ⁺²¹, EAPCD20, EAPCD21, KMH⁺²⁰, dRNS21, Ole20, Ole21, PMGR⁺²¹, RYC⁺²⁰, SZMM22, XQJ⁺²¹, YZY⁺²²]. **dimer** [RNRBFC21, SFB20]. **dimeric** [ZPS⁺²⁰]. **dimerization** [CMY22, GOS20, HYHW22]. **dimers** [LK20, ZLT⁺²⁰]. **dimethyl** [KMK21].

dimethylaminophenyl [BRB⁺21]. **dimethylcyclohex** [BRB⁺21].
dimethylcyclohexane [BZW⁺21]. **dimethylcyclohexyl** [BWLZ22].
dinitrogen [Kov20]. **diodes** [LK20]. **dione** [LZS20]. **dioxide**
 [GG20a, HLL20a, KWWZ20]. **dioxin** [ARBM21]. **dioxin-like** [ARBM21].
dioxygen [DTAS21]. **Dipole**
 [WWKH22, ACM20, BCM⁺22, CZ21, HTNP21]. **Dirac** [CRC21]. **direct**
 [WLY⁺20]. **directed** [WSSD21]. **Dirichlet** [Ole20, Ole21]. **Discerning**
 [MAMB⁺22]. **discovery** [GKK21, HBY20]. **discrepancy** [ID21]. **discrete**
 [TPCSD20]. **discussion** [Yos20]. **disease** [ZLH20a]. **dislocation** [BU20].
dispersion [BSH⁺21, GMO⁺20]. **dispersion-corrected** [GMO⁺20].
dissociation [BZW⁺20, GRLH21, MM21, ZZLY22]. **dissociations**
 [JWZZ20]. **Distance** [LAAP21, RMWF20]. **distant** [DTAS21]. **distortions**
 [PZGH⁺20]. **distribution** [BRF21, CSS⁺21, Gun21, MFC20a, RPT21b].
distributions [SDK⁺21]. **disubstituted** [MSADA21]. **disulfide**
 [AKK⁺21, PD22]. **disulfide/thiolate** [PD22]. **disulfides** [PD22, RK21].
dithiafulvene [ZKP22]. **dithiophene** [XPZ20]. **diverse** [WLH⁺20]. **DMRG**
 [WFG⁺21]. **DMSO** [VOK⁺20]. **Do** [AS22, LFMG20]. **dodecaboride**
 [YFX⁺22]. **dodecaborides** [PJ20a]. **dodecahedrane** [Ari21]. **Does**
 [LK20, RRSF22]. **domain** [GG20b, MJRS20]. **donating** [XZ20]. **donor**
 [BSS21, CLL20, CZW21, DSNZ⁺20, LFRTRP⁺20, LYT⁺20, XZ20]. **donor-**
LYT⁺20. **donor-acceptor** [BSS21, LFRTRP⁺20]. **donor-bridge-acceptor**
 [CZW21]. **donors** [CLL20, LL21, XPZ20, ZZ22]. **dopant**
 [LXWZ21, ZCL⁺22]. **doped** [DYG21, ER22, GYC20, KS21, MKKK22,
 MCP⁺20, MAHRA⁺21, MIM21, MTA⁺22, Pan20, RBJ21, RINHY20,
 SDL⁺22, THS20, VKS21, WWM⁺21, XWS⁺22]. **doped-carbon**
 [EGLJQ⁺21]. **doping** [GG20a, GRZ⁺21, KM21a, MHS21, MNWD20,
 RHS⁺21, RDMF21, WLY⁺20, YCPW20, ZZZ20b]. **dosimetry** [JAZ⁺20]. **dot**
 [BU20, BUKA21, Bah22, KB21, MIM21]. **dots** [Mok21a, Ole21, RMM⁺22].
double [AAN⁺21, ARRB⁺21, HMBPJ⁺20, KRB20, RCM⁺22, RKA⁺21,
 ZFB⁺20, ZX21, ZCL⁺22, ZZL⁺20a, GSMT⁺20]. **double-hybrid**
 [HMBPJ⁺20]. **doubles** [BBG20, dSFdSdMdM20]. **doubly**
 [ATL⁺20, KKH21, WWKH22]. **dppz** [DSNZ⁺20]. **dppz-based** [DSNZ⁺20].
DR [TCL⁺21]. **DR-2** [TCL⁺21]. **dragged** [PMdN21]. **dragging** [KAUB21].
DRCNnT [WZ20]. **dressed** [Dau21, HSV22]. **driven**
 [CDG⁺21, KRB20, TSN⁺21, WAM⁺20]. **driving** [CCZ20]. **drug**
 [LAAP21, MJA20, PSJ22]. **drugs** [Hav21, KAA21]. **dry** [HYC⁺21, RSD21].
dual [NHNO20]. **during** [FCL22]. **dye**
 [FZL⁺20, MSKA20, PIA21, PGPHAPM20, SIA20, YLL⁺20]. **dye-sensitized**
 [FZL⁺20, MSKA20, PIA21, PGPHAPM20]. **dyes**
 [FZL⁺20, MSKA21, MKuAS⁺22, MRI20, PIA21, PGPHAPM20]. **Dynamic**
 [NHNO20, ATL⁺20, CMM21, SFB20]. **Dynamical** [HL20, BPB⁺20].
Dynamics [PMdN21, CLS⁺22, DKK⁺20, Doh20, GRLH21, INV22b, JAZ⁺20,
 LLC20, MZD⁺20, MW21, MKD21, Mok21c, dAOdASP⁺20, RSBK20, RKI20,
 RKG21, SASA21, TSN⁺21, TCL⁺21, TCX⁺22, WV20b, WAM⁺20, ZKP22].

E-2 [SYT⁺21]. **E/Z** [HYHW22]. **E/Z-HFO-1234ze** [HYHW22]. **e26221** [Sur22]. **e26530** [Ano22a]. **earth** [LL21, MBKA21, MCP⁺20, NG20]. **easy** [GKK21]. **Eccentricity** [ZMS21, WYZZ20]. **Eccentricity-based** [ZMS21]. **edge** [RG20, RNA22, IAI20]. **edged** [DJC21]. **Editorial** [SSL22]. **education** [MNN⁺20, Shi20]. **Effect** [BPB⁺20, JBPV21, LQZ⁺21, NG20, SCAD⁺20, SFB20, WCZ⁺20, BGK⁺22, BA21, CRKMC21, CLC⁺21, CLLC21, GN21b, HL20, JHH⁺22, KRS⁺21, KAUB21, LYT⁺20, LSS⁺21, LXWZ21, MSM⁺20, MKM⁺20, MTA⁺22, MHD20, NIA21, PVR20, QDC⁺22, TPT20, WXLL21, YZD⁺21, YCSK20, ZZZ20b, DTAS21, EM21]. **effective** [DFB20, KAG⁺20, MZT20, VKK⁺21]. **Effects** [HDF⁺21, RHS⁺21, Wan21, YLL⁺20, YZL21a, BZW⁺20, DKK⁺20, FPdS21, HOVG20b, HLL20b, JIFM22, KSP20, LZL⁺21, MKuAS⁺22, MHS21, OAJ21, ONH⁺21, QdOdMC⁺21, RKI20, SSIE21, SSEI21, STN20, SP20b, WZ20, WDS⁺20, WXLL21, WLLS21, YCPW20, ZIA20, ZL21, ZCL⁺22, ZGCF20, tZNB⁺22]. **Efficiency** [TCSG⁺20, KMH⁺20, SIA21]. **Efficient** [KLT21, BA21, FZL⁺20, FAJOF20, RKA⁺21, RINHY20, SYL⁺21, WP22]. **eigensolver** [GDR21]. **eigensystem** [DS20]. **Einstein** [PMdN21]. **elastic** [BA22a, GGUU21, LWH⁺21, MSS22, MBM⁺21, SDK⁺21, SG20]. **elasticity** [YFX⁺22]. **Electric** [ZXS20, AMM21, CWY⁺20, EM21, LNX⁺21, LCP21, MKM⁺20, Mok21a, NYX⁺21, RYC⁺20, TWT⁺21, VM20, WWZ⁺21, WP22, ZIA20, ZYZ⁺21a]. **electrical** [Rac21]. **electride** [PC22, TSW⁺20]. **electrochemical** [MHS21, XQJ⁺21]. **electrochemotherapy** [ZYZ⁺21a]. **electrode** [dRNS21, SUG20, XWS⁺22]. **electrodynamics** [SI20]. **Electron** [BA22a, DSNZ⁺20, SP20b, SA20, CCZ20, CPL⁺21, CLL20, CZW21, Cio22, FFBH21, Hua20, JVK22, JXM22, KZ21, LNE⁺20, LZ20, LL21, Lom21, LFMG20, MSS22, MSKA20, MSADA21, PT21, PJ20b, QOM⁺20, Rad21, SDS19, SDS20, SCAD⁺20, STT20, TWT⁺21, XZ20, YÇDÖ21, ZIA20, ZS21, ZGCF20]. **electron-correlation** [ZIA20]. **electron-deficient** [LZ20]. **electron-donating** [XZ20]. **Electron-donor** [DSNZ⁺20]. **electron-hole** [CPL⁺21]. **electron-transfer** [TWT⁺21]. **electron-withdrawing** [FFBH21, SCAD⁺20]. **Electronic** [CSY⁺21, DJC21, FK20, MCP⁺20, RKA⁺21, RNFMC20, SBA21, Üng20, ZYZ⁺22, ZIA20, BPB⁺20, BBAA21, BA21, BWBR21, CMGH⁺21, CLLC21, DDSB22, Dau21, DCY21, FPdS21, FH21, GYC20, GRZ⁺21, GGUU21, Gun21, HNO⁺21, INV22b, JZX⁺20, KKH21, KYL⁺20, KK21, KLK21, KM21b, KMG22, LLZC20, sLhZX⁺22, LWH⁺21, MKKK22, MKuAS⁺22, MKM⁺20, MKD21, MK21, MIM21, MM21, MBM⁺21, MEWD20, NLA⁺21, ORL⁺20a, ONH⁺21, OMA21, Pan20, Pan22, RPT21b, SBG21, SCU21, dOSdASC⁺20, SG20, TMH21, TT21b, TVdVN21, TVdVN22, UBV⁺21, WXL⁺21, WP20, WFG⁺21, XFW⁺20, XBK⁺20, XWS⁺22, YLL⁺20, YCPW20, ZLH⁺20b, ZZZ20b, ZHFD⁺20, tZNB⁺22]. **electronic/atomic** [UBV⁺21]. **electronic/atomic-scale** [UBV⁺21]. **electrons** [CFJ20, PJ20b, Sah21, SDK⁺21, TWT⁺21]. **electrophilic** [KZ21]. **electrophilicity** [JPSC20]. **electrostatic** [ABS20, Doh20, SSIE20, ZGCF20].

element [CMGH⁺²¹, WWLL21]. **elements** [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, DG21, Hua20]. **embedding** [Doh20, HOVG20b, Höf21, JMOW20, MJRS20, OAJ21, SMJ20, WP20]. **embedding-based** [SMJ20]. **Emergences** [KOB20]. **emission** [SCZ21]. **emissive** [DSNZ⁺²⁰]. **emitter** [SYL⁺²¹]. **emitting** [LK20]. **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]. **energetic** [JXL⁺²¹, PLT⁺²⁰, WJL⁺²¹, XWJ⁺²¹, ZJW⁺²¹]. **energetics** [ÜB20]. **energies** [AIB21, BBG20, dSFdSdMdM20, FH21, GRFM20, HMBPJ⁺²⁰, JXM22, LCP21, MFC20a, OB21b, PPCF⁺²⁰, STN20, SPR22, TTH20, TdV21, VCM⁺²¹]. **Energy** [YÇDÖ21, AIB21, AB21, CZ21, CZW21, HTNP21, HW21a, JHH⁺²², KRS⁺²¹, MC22, MZ21, MHD20, NF20, NR21, OR21, PT21, PZGH⁺²⁰, RRD⁺²², RKA⁺²¹, RK21, SFPH22, SPR21, SCU21, SKG21, VP20, WP22, XWLZ20, ZJW⁺²¹, ZZXT21, Zhu21]. **Engaging** [BHH20]. **engineering** [Cio22, JHH⁺²², PIA21]. **enhance** [GRZ⁺²¹, JHH⁺²²]. **Enhanced** [AAB22, AJC⁺²¹, EGLJQ⁺²¹, FSR⁺²², SN21, WLY⁺²⁰]. **Enhancement** [BSS21, PVR20, VdM22, YCL⁺²²]. **enol** [KMK21, LZS20, SLdS20]. **ensemble** [LMA21, SF20a]. **ensembles** [CN21]. **entanglement** [AkAR⁺²¹]. **enthalpy** [WWL21]. **entropic** [KRB20]. **entropies** [IRA⁺²⁰, NZAH21, Ole20, SD20, TPCSD20]. **entropy** [AIN⁺²⁰, EAPCD20, JSF⁺²¹, MSA22, RNA22, SJ20, SLPS20]. **envelope** [Dau21, GZCY22]. **environment** [BMF20, DFB20, STN20]. **environmental** [XHX⁺²⁰, YZD⁺²⁰]. **environments** [CLS⁺²², CBB21]. **enylidene** [BRB⁺²¹]. **enynes** [YYL21, ZZZW20]. **EPc** [PC22]. **Epoxidation** [CSY⁺²¹, AAN⁺²¹, WLP⁺²⁰]. **equation** [BBG20, CSS⁺²¹, Eti20, HRA⁺²², Izs21, LBP20, NACP21, OO21a, PM22, SS21]. **equation-of-motion** [BBG20, Eti20]. **equations** [KLT21, SD20, TJA20]. **equilibrium** [BM21, EM21, KMK21, SP20a]. **equivalent** [LLZ⁺²⁰]. **Erratum** [Ano22a, Bah22, Sur22]. **error** [DK21, SM22]. **error-free** [SM22]. **errors** [LCP21]. **estimate** [GG20b]. **Estrada** [LXZ21b]. **ethanol** [BTS⁺²¹, MFC20b]. **ethanol-to-butadiene** [BTS⁺²¹]. **ethers** [CMM⁺²², TT21a]. **ethyl** [YLL⁺²⁰]. **ethylene** [YZD⁺²¹]. **Europium** [DCY21]. **Europium-linked** [DCY21]. **EuRu** [KMG22]. **EuSi** [DCY21]. **Ev** [RNB22]. **Ev-degree** [RNB22]. **Evaluation** [VL21, BM21, ÖÇÖ21, Pev21, RDMF21, SSIE20, VKK⁺²¹]. **even** [WZ20]. **Evidence** [Hol21]. **evolution** [ASO⁺²², AKP22, DLZ⁺²¹, GYC20, LFMG20, ORL^{+20b}, RSBK20]. **Exact** [CWY⁺²⁰, GN20, KRS⁺²¹]. **examination** [ASHPHCB20]. **Examining**

[BMH21]. **example** [SBM22, dOSdASC+20]. **excellent** [WDS+20].
exceptional [Shi20]. **excess** [TWT+21]. **Exchange**
[MMM20, Cin20, KRS+21, KA21, MMM16, NHNO20, ZPS+20]. **excimer**
[LK20]. **excitation** [BZW+20, FK20, HMBPJ+20, JBPV21, STN20].
excitations [BMF20, GDR21]. **excited** [BXWK22, DFB20, Eti20, FK20,
HL20, Izs21, KGSD20, LBG20, Mka20, Nag20b, NZ20, NYX+21, Rui22,
SBG21, SKG21, TVdVN22, WY20, WWKH22]. **excited-state**
[Eti20, Nag20b]. **exciton** [BZW+20, CZ21, LYTS20]. **exhibition** [MOB21].
expanded [Cha21b]. **expansion** [GM21, RSBK20]. **expansions** [SMJ20].
expectation [HTNP21, JIFM22, ZHJ+20]. **expected** [FYL21]. **experiment**
[ID21]. **Experimental** [LZS20, TCL+21, BBG20, LSS+21, PPCF+20,
RINHY20, WWZ+20, WAW+21, YHZ+22]. **explain** [RRSF22]. **explanation**
[LAKJ20]. **explicitly** [JIFM22, Var21]. **Exploiting** [HRA+22]. **exploration**
[BWLZ22, DYG21, Kan21, LZZ+20, Röh21]. **Exploring**
[DDSB22, EGLJQ+21, FSR+22, SKG21, WZ20, ZGCF20, ZZ22, ZWL22].
explosive [HRTSS+20, MWC+21, WDS+20, ZGCF20]. **explosives**
[WJL+21]. **exponential** [PGROM20, PMGR+21, XJ20]. **exponential-type**
[PGROM20, PMGR+21, XJ20]. **Exponentially** [SPR21, SPR22].
exponentials [Lom21]. **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 [HYC+21, TCX+22, WWZ+20, YHW+22, YHZ+22].
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, PVR20, TWT+21, Yan20, MBKA21, ÉC21, GZC21, MKD21,
MNWD20, NZ20]. **f-orbital-dependent** [MBKA21]. **f12** [VKK+21]. **Face**
[DQS+21]. **fail** [RRSF22]. **family** [WJL+21, XWLZ20, XWJ+21]. **Fan**
[NR21]. **fast** [GKK21]. **Fatigue** [NYX+21]. **FCIQMC** [WFG+21]. **Fe**
[MIM21, SKR+21, SUG20, WFG+21]. **Feature**
[HNO+21, CSY+21, JVK22, WWLL21]. **Feature-rich** [HNO+21]. **features**
[MK21, Mok21a]. **FeCrSe** [PKBZ20]. **FeCrTe** [PKBZ20]. **feedback**
[GOR20]. **Feinberg** [NACP21, OO21b, OO21a]. **feldspar** [HYY20]. **FeNC**
[GKPK21]. **fermions** [LMMA21]. **ferrate** [CSY+21]. **ferrimagnetism**
[LHL+21]. **ferrocene** [WV20b]. **Ferrocenes** [Cha21a]. **ferroelectric**
[MAHRA+21]. **ferromagnetic** [AMK+20, SG21]. **Ferromagnetism**
[MNWD20]. **FeSi** [TMH21]. **Field**
[ZXS20, ACM20, AMM21, CRC21, CFJ20, CWY+20, Dau21, EM21, GN21b,
GOR20, HK22, HP21, KKH21, LNX+21, LCP21, MKM+20, Mok21a, NIA21,
PPR21, SM22, TSN+21, TWT+21, WP22, ZIA20]. **field-dressed** [Dau21].
field-effect [NIA21]. **Field-Phenyl** [ZXS20]. **fields**
[Bah22, Bra21, KB21, NYX+21, RYC+20, VM20, WWZ+21, ZYZ+21a]. **fifth**
[Cio22]. **fifth-order** [Cio22]. **figure** [RMLPGHP20]. **filled** [KMG22]. **fine**

[ZHJ⁺20]. **finite** [VL21]. **finite-difference** [VL21]. **fire** [HYC⁺21, TCX⁺22, WWZ⁺20, YHW⁺22, YHZ⁺22]. **fire-extinguishing** [TCX⁺22, WWZ⁺20, YHW⁺22, YHZ⁺22]. **First** [FMH⁺22, GSRG22, GGUU21, Kan21, KA21, KHH⁺21, LHL⁺21, LXWZ21, MBKA21, MHS21, OGSPP⁺22, Pan20, PM22, RMeH⁺20, RED21, UV20, WXL⁺21, WWM⁺21, XCZ⁺21, YZL⁺21b, ZRR⁺21, AJC⁺21, AKKN20, BA22a, DLZ⁺21, DAR⁺21, ER22, HL20, JZX⁺20, JXM22, Kan22, KMG22, sLLqX⁺20, LYT⁺20, LWH⁺21, MSKA21, MAHRA⁺21, MBM⁺21, MNWD20, NF20, NZ20, PL20, RS21, RNFMC20, SFT⁺21b, SG21, 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, XFW⁺20]. **First-principles** [GSRG22, Kan21, KHH⁺21, LHL⁺21, LXWZ21, MBKA21, OGSPP⁺22, Pan20, RED21, WWM⁺21, XCZ⁺21, YZL⁺21b, ZRR⁺21, AJC⁺21, AKKN20, DLZ⁺21, ER22, JZX⁺20, Kan22, KMG22, LWH⁺21, MSKA21, MAHRA⁺21, PL20, RS21, SFT⁺21b, ZLH⁺20b, tZNb⁺22]. **first-row** [JXM22]. **Fisher** [NACP21, OO21b, AkAR⁺21, AIN⁺20, Nag22, OO21a]. **fit** [PJ20b]. **fitted** [Boz21]. **Fitting** [Pev21]. **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** [SYL⁺21]. **fluorescent** [GA20, LXZ⁺21a, LYTS20, TSHRS⁺20, ZLH20a]. **fluoride** [LZL⁺21]. **fluorides** [SP20b]. **fluorine** [HNO⁺21]. **fluorine-** [HNO⁺21]. **fluorographene** [ID21]. **fluorouracil** [BSH⁺21]. **flutamide** [PSJ22]. **flux** [BM21]. **Fock** [JBPV21, RPT21a, RPT21b, Rui22]. **Fock-space** [JBPV21]. **force** [Bra21, CCZ20, JD20, PPR21]. **forecasting** [AkAR⁺21]. **form** [BRHECY⁺22, LK20, MWBQ20]. **formalism** [AMM21, Eti20, MM22a]. **formamide** [SE20]. **Formamidinium** [ZCL⁺22, PAS⁺21]. **Formation** [SV21, WJF⁺21, LRG⁺20, LLW⁺21, SFB20, SBG21, WWL21, WZL⁺21]. **formic** [SDL⁺22]. **forms** [KMK21]. **formulation** [BM21]. **Fourier** [SS21]. **FOX** [ZZLY22]. **FOX-7** [ZZLY22]. **Fractional** [Mos21, SD20]. **fragility** [JD20]. **fragment** [DFB20, NF20, PNC20]. **frame** [HTNP21]. **framework** [Boz21, HTNP21, HRTSS⁺20, HRA⁺22, SBA21]. **frameworks** [HW21a]. **free** [AKKN20, CPK22, dSFdSdMm20, HZC21, Nag20b, PIA21, PPCF⁺20, SM22]. **free-standing** [HZC21]. **freedom** [Wan21]. **friendly** [GPP⁺21]. **Frontier** [SP20a]. **Frozen** [SMJ20, Höf21, OAJ21]. **Frozen-density** [SMJ20, Höf21]. **frustrated** [SSIE20]. **full** [LHL⁺21, SG21]. **full-Heusler** [LHL⁺21]. **full-Heuslers** [SG21]. **fullerene** [CRKMC21, DFK20, DYK22, GXL⁺22, GMO⁺20, GMRKMCMC21, SBM22, VKS21, dPZFM⁺22]. **fullerene-ZnPc** [CRKMC21]. **fullerenes** [GMRKMCMC21]. **Fully** [MSS22]. **function** [DS20, NZ20, Sør21, SY21, Sur20, Sur22, WWM⁺21]. **Functional** [BVL22, ABDD22, ARRB⁺21, BBAA21, BZP⁺20, BA21, BRB⁺21, BB20, BSH⁺21, CXZ⁺21, CPL⁺21, DRV20, DPC⁺20, DFK20, EGLJQ⁺21, EB22,

FFBH21, GMO⁺²⁰, GTV20, JZL⁺²¹, KRS⁺²¹, KVCS21, KYL⁺²⁰, KAG⁺²⁰, LLW⁺²¹, LK21, LFRTRP⁺²⁰, LCP21, LSS⁺²¹, MSKA20, MKKK22, MR21, MIM21, MOB21, MP20, Nag20b, Nag22, NHNO20, PM22, PJ20b, PD22, Pev21, QdOdMC⁺²¹, QOM⁺²⁰, RSD21, Röh21, SSEI21, SPF⁺²², SK20, STN20, SK21, SF20a, Shi21, SBJ20, SG20, STF21, TXW⁺²⁰, THL⁺²¹, TCX⁺²², VGSS20, WZ20, XZ20, XQJ⁺²¹, XWS⁺²², YZD⁺²¹, ZZZ^{+20a}, ZZLC20, ZXS21, dPZFM⁺²²). **functionalized** [CSY⁺²¹, XZ20]. **functionals** [BXWK22, HMBPJ⁺²⁰, Pev21, ZYZ⁺²²]. **functioning** [TPT20]. **functions** [CPK22, Gun21, TVdVN21, TVdVN22]. **fundamentals** [CM21]. **fused** [PVR20]. **Future** [KKRR21, JHH⁺²²].

g [RINHY20]. **g-C** [RINHY20]. **Ga** [GSRG22, MBM⁺²¹, NG20, Yan20, sLLqX⁺²⁰]. **Ga/In** [GSRG22]. **gap** [OR21, RK21, SCU21, WWLL21, WLY⁺²⁰]. **gas** [AN20, GOS20, LZL⁺²¹, PT21, RKI20, SASA21, Shi21, TTTH20, VdM22]. **gas-** [RKI20]. **gas-phase** [GOS20, LZL⁺²¹, SASA21, VdM22]. **gases** [dAOdASP⁺²⁰]. **gate** [TPT20]. **Gaussian** [Sha20]. **Gaussian-type** [Sha20]. **Gaussians** [JIFM22]. **Gd** [NG20]. **General** [Ano22a, BT21, KH20, OB21b, TdV21]. **Generalized** [GN21a, GDR21, MZT20, GRFM20, HJIO21, IRA⁺²⁰, WFG⁺²¹, WP22, ZHJ⁺²⁰]. **Generation** [KYL⁺²⁰, GW21, LYW⁺²⁰, VSKG21, WAM⁺²⁰]. **generative** [HBY20]. **genetic** [RSBK20]. **Geometric** [RRS21, BDEM21, GRLH21]. **geometric-arithmetic** [BDEM21]. **geometrical** [ZZZ20b]. **geometries** [SP20a]. **geometry** [CN21]. **Germany** [KKRR21]. **GIAO** [GZC21]. **glassy** [MZD⁺²⁰]. **Global** [ZG21, DYG21, KYL⁺²⁰, TCL⁺²¹]. **globular** [Ye20]. **glutathione** [KI20]. **glycerol** [SBJ20]. **glycerol/hydrogen** [SBJ20]. **glycinamide** [ES21]. **glycine** [GOS20]. **glycolaldehyde** [ZWW⁺²²]. **gmx2qmmm** [GPP⁺²¹]. **go** [GTV20]. **gold** [QOM⁺²⁰]. **good** [Rac21]. **Gourava** [SZMM22]. **governing** [KLT21]. **gradient** [AMM21]. **gradients** [LCP21]. **graduate** [CM21]. **graph** [AIAG21, AD22, CLW21, IAI20, LS21, RKI20]. **graph-theoretically** [RKI20]. **graphene** [ARBM21, DJC21, ID21, LZSA20, LK21, LXWZ21, MI20, QDC⁺²², RMM⁺²², RBJ21, SPF⁺²², SDL⁺²², YZL21a]. **Graphitic** [LFX⁺²¹, YCPW20]. **graphs** [Ano22a, AD22, BDEM21, BT21, CL21, FYL21, Hao21, LCX⁺²¹, RRS21, RA20, WYZZ20]. **graphyne** [DRV20, HDF⁺²¹, 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, KDY⁺²², LLMQ20, PGPHAPM20, TT21b, YLL⁺²⁰]. **group-11** [Cha21b]. **group-14** [KDY⁺²²]. **Group-IV-based** [STF21]. **groups** [LFRTRP⁺²⁰, XZ20]. **growth** [DYK22, DYG21, FCL22, BRB⁺²¹]. **guess** [HK22]. **GYs** [HDF⁺²¹].

H [ASO⁺22, Ari21, EB22, FK20, GNC20, JWZZ20, MOB21, PVR20, Shi21, SRS21, ÜB20, WCZ⁺20, WAW⁺21, YCSK20, Cha21a, CLS⁺22, DKK⁺20, Dau21, KDY⁺22, LZL⁺21, MSS20, dAOdASP⁺20, ÖÇÖ21, Roy20, SSIE20, SSIE21, SSK20, STF21, WY20, WXL⁺21, WZL⁺21, WSSD21, WHYL21, YZD⁺21]. **H-bond** [ÖÇÖ21]. **H-like** [CLS⁺22]. **H/D** [DKK⁺20]. **Half** [PKBZ20, Rui22, BB20, HBB⁺21, KDY⁺22, LHL⁺21, ONH⁺21, RCM⁺22, SG21, ZRR⁺21]. **half-Heusler** [PKBZ20, RCM⁺22, ZRR⁺21]. **half-metallic** [BB20, LHL⁺21, ONH⁺21, SG21]. **Half-metallicity** [PKBZ20]. **Half-Projected** [Rui22]. **half-sandwich** [KDY⁺22]. **halide** [AAM⁺20, BPB⁺20, PAS⁺21, ZZLC20]. **halides** [CFM⁺21, LL21]. **halogen** [KSP20, WXLL21]. **Halon** [YHW⁺22]. **Hamiltonian** [AKP22, SM22]. **hard** [MR21]. **hardness** [PJ20a]. **hardware** [RBSW21b]. **harmonic** [RNFMC20]. **Hartree** [RPT21a, RPT21b, Rui22]. **HC** [PAS⁺21]. **HCl** [WY20, CMM⁺22, WY20]. **HCl-catalyzed** [CMM⁺22]. **HCNO** [MM20]. **He-like** [TVdVN21, TVdVN22]. **heavier** [KDY⁺22, ZLT⁺20]. **heavy** [CFM⁺21]. **HeH** [MM21, Wan21]. **Heisenberg** [CSK21, JVK22]. **helicity** [XAM⁺22]. **helium** [CBB21, DG21, LBG20, MF21a, NZAH21, SPR21, TVdVN22]. **helium-like** [NZAH21]. **helix** [ZXS21]. **Hermitian** [HRA⁺22, LMA21, SM22]. **hetero** [JS21]. **heterocycle** [WJL⁺21]. **heterocycle-based** [WJL⁺21]. **heterocycles** [SSEI21]. **heterocyclic** [DDSB22, JRA21, LLZ⁺20, LLMQ20, PM20, SCAD⁺20, YLL⁺20, ZFB⁺20]. **heterodinuclear** [ZXS21]. **heterogeneous** [PGÁML21, WLP⁺20]. **heterogeneous-homogeneous** [WLP⁺20]. **heterojunction** [BZW⁺20, MI20]. **heterostructures** [OGSPP⁺22]. **Heusler** [BB20, GGUU21, HBB⁺21, 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** [WWZ⁺20]. **hexagonal** [BMR21, CPL⁺21, CDR20, DQS⁺21, FYL21, RMLPGHP20, SZMM22, ZFB⁺20]. **hexamer** [MFC20b]. **hexanitro** [ZGCF20]. **Hf** [GGUU21, LLZC20]. **HFO** [HYHW22]. **HFP** [SK20]. **HfSe** [OGSPP⁺22]. **HfSSe** [OGSPP⁺22]. **HfTaZrNb** [JSF⁺21]. **HfTaZrTi** [JSF⁺21]. **Hg** [QOM⁺20, FAJOF20]. **Hierarchical** [TJA20]. **High** [LYT⁺20, XFW⁺20, XJLH21, GZWL22, HLL20a, HW21a, JSF⁺21, KMH⁺20, LFX⁺21, MZ21, PJ20a, Rac21, SF20b, ÜB20, XWLZ20, ZJW⁺21, ZLT⁺20, 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]. **higher** [BXWK22]. **Highly** [GG20a, PAS⁺21, SC21]. **history** [AB21, Rui22]. **HMDSO** [HCZ20]. **HNO** [WZL⁺21]. **HNSO** [MSS20]. **hole** [CPL⁺21, HLL20b, KSP20, LZ20, LL21, VM20, ZL21, ZZ22]. **hole-transporting** [LZ20]. **holmium** [DYG21]. **holmium-doped** [DYG21]. **homogeneous** [PT21, WLP⁺20]. **homolytic** [KAG⁺20]. **homonuclear**

[BA22b]. **honeycomb** [tZn^{b+22}]. **Horodecki** [NACP21, OO21b, OO21a]. **HoSi** [DYG21]. **hosts** [CRKMC21]. **hot** [CLS⁺²², LYTS20]. **HRPA** [JS21]. **HS** [ZZZ^{+20a}]. **Hückel** [WWKH22]. **hybrid** [BGK⁺²², HMBPJ⁺²⁰, WZ21]. **hydrated** [SK20]. **hydrates** [ZLH^{+20b}]. **hydration** [LK21]. **hydride** [WJF⁺²¹]. **hydrides** [RMeH⁺²⁰]. **hydroarylation** [LG21]. **hydroboration** [SSIE21]. **hydrocarbons** [LCX⁺²¹, LPH22, WYZZ20]. **hydrochalcogenation** [JRA21]. **hydrochlorination** [AKKN20]. **Hydrogen** [dAOdASP⁺²⁰, SK20, BMF20, CSY⁺²¹, DLZ⁺²¹, EAPCD20, EAPCD21, FGMO20, JVK22, JXYL20, KHH⁺²¹, KLT21, LAKJ20, LWC⁺²¹, LYW⁺²⁰, RS21, RMeH⁺²⁰, RDMF21, SI20, SFB20, SRH20, SBJ20, XJLH21, STI20]. **hydrogen-like** [JVK22, XJLH21]. **Hydrogen/** [STI20]. **hydrogenation** [LSS⁺²¹]. **hydrogenic** [SLPS20, TPCSD20]. **hydrogenlike** [WKH20]. **hydrolase** [ÖÇÖ21]. **Hydrolysis** [MSS20, LZL⁺²¹, SASA21, ZZL^{+20a}]. **Hydrolytic** [UAH⁺²⁰]. **hydrophobicity** [JPSC20]. **hydrosilylation** [ZXS20]. **hydrothermal** [FCL22]. **hydroxide** [SKR⁺²¹]. **hydroxyacetone** [JD20]. **hydroxyl** [SYT⁺²¹]. **hydroxymethylfurfural** [LSS⁺²¹]. **hydroxyphenyl** [KMK21, PPR21]. **hydroxyquinoline** [SFPH22]. **Hylleraas** [BXWK22, SPR21, SPR22, ZGJ⁺²⁰]. **Hylleraas-configuration** [SPR21, SPR22]. **hyperbolic** [IRA⁺²⁰]. **hyperfine** [JAZ⁺²⁰, ZHJ⁺²⁰]. **hypergraphs** [LXZ21b, ZZL20b]. **hyperpolarizabilities** [LYT⁺²⁰, MCP⁺²⁰]. **hyperpolarizability** [BMF20]. **hypertrees** [Zhu21]. **hypoxanthine** [ES21].

Identification [HCZ20, SI20]. II

[LLMQ20, PPR21, WFG⁺²¹, ES21, PD22, SPR22, TVdVN22, ZPS⁺²⁰]. **III** [DSNZ⁺²⁰, LLW⁺²¹, RKG21, VSKG21, WLH⁺²⁰]. **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]. **imidazole** [KMK21]. **impact** [MSS22]. **impenetrable** [YÇDÖ21]. **Implementation** [ZMJ⁺²⁰, ABS20, Pon19, TPB⁺²⁰, Yos20, ZS21]. **implication** [MM21]. **imposed** [WY20]. **improve** [BXWK22, GZC21, MSKA20]. **Improved** [FFBH21, XJ20, CPK22, GG20a, HJIO21, NR21]. **improvement** [MSKA21]. **Improving** [BBG20, dPZFM⁺²²]. **impurity** [ZYZ^{+21b}]. **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]. **index**

[AIAG21, ADZA21, BDEM21, BMR21, DQS⁺21, GN21a, IAI20, IMJ21b, LPH22, LXZ21b, WYZZ20, ZZL20b]. **indices** [AII21, Ali20, Ano22a, BT21, CSGR21, DL21, DTW21, DAR⁺21, FYL21, Hav21, IMJ21a, Jah20, KAA21, LSG21, LAAP21, LCX⁺21, MAK⁺22, RNB22, RA20, RMWF20, Ye20]. **indirect** [OR21, WLY⁺20]. **indirect-to-direct** [WLY⁺20]. **indole** [WSSD21]. **Induced** [CPL⁺21, BUF⁺22, CBB21, KGSD20, MNWD20, PM20, SYL⁺21, YCL⁺22]. **Influence** [BS20, CZW21, MIM21, MT21, PL20, WZL⁺21, BCM⁺22, BRHECY⁺22, CCZ20, CYJC20, CZ21, GYC20, 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, LMA21, TAS21, AkAR⁺21, AIN⁺20, IRA⁺20, KRB20, MF21a, Nag20b, Nag22, NACP21, NZAH21, 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]. **initiated** [YZD⁺20, YST⁺21]. **initiation** [CLC⁺21]. **initio** [BZW⁺21, CMGH⁺21, HZC21, JAZ⁺20, JSF⁺21, MZD⁺20, ORL⁺20b, PASS21, RKI20, RKG21, SASA21, ZLT⁺20, ZKP22, ZHS21]. **injection** [CPL⁺21, MSKA20]. **inlets** [CDR20]. **Innovation** [GG22]. **inorganic** [ZZLC20]. **insertion** [SN21]. **insertion-enhanced** [SN21]. **Insight** [ARRB⁺21, BZP⁺20, BWBR21, HMN20, NIA21, SIA21, SSEI21, ZPS⁺20, BSS21, MSM⁺20, MWBQ20, Pan22, RG20, SCU21, VKS21, WLH⁺20, WHYL21, ZYZ⁺21a, ZZ22]. **Insights** [PGPHAPM20, QOM⁺20, ZGCF20, ABDD22, FAJOF20, LZS20, LXZ⁺21a, MNWD20, RBJ21, RYC⁺20, SYL⁺21, WSSD21, WFG⁺21, GMO⁺20]. **instantly** [BXWK22]. **Institute** [MNN⁺20]. **institution** [SF20b]. **insulator** [CRC21]. **Int** [GM21, Sur22]. **integral** [BM21, DKK⁺20]. **integrals** [Boz21, GM21]. **Inter** [TWT⁺21]. **Inter-cage** [TWT⁺21]. **Interaction** [BSH⁺21, ATL⁺20, AIB21, AB21, BVL22, CBB21, dSFdSdMdM20, MM22a, MKD21, PSJ22, Rad21, RED21, SPR21, SPR22, ZXS20, ZGJ⁺20, dLRdLJ⁺20]. **interaction-induced** [CBB21]. **Interactions** [MWBQ20, KA21, MC22, MF21b, MM21, NHNO20, OGT20, dAOdASP⁺20, SK20, SC21, UP20, WWWC21, ZKP22]. **interconversion** [PD22]. **interconversions** [HYY20]. **Interface** [BZW⁺20, GPP⁺21, KAUB21, UBW⁺22]. **interference** [BA22b]. **intermediate** [QOM⁺20, SKR⁺21]. **intermetallic** [BBAA21, sLLqX⁺20].

intermolecular [Kid21]. **internal** [Bra21, VM20]. **Interpretation** [AIB21].
intersections [MM20, WAM⁺20]. **intersystem** [KWWZ20, LYTS20, SV21].
intra [ZZXT21]. **intra-annular** [ZZXT21]. **Intramolecular**
 [JD20, CCZ20, SSIE20, YCSK20]. **Intriguing** [HBY20]. **Introducing**
 [Sur20, Sur22]. **introduction** [Nat22]. **invariants** [NS22, ZMS21]. **inverse**
 [LACP21, NG20, VN21]. **Inversion**
 [MMM20, BZW⁺21, Cin20, KH20, LLZ⁺20, MMM16].
inversion-topomerization [BZW⁺21]. **Inverted** [YCSK20]. **Inverting**
 [PJ20b]. **investigate** [THS20, ZRR⁺21]. **investigated** [KAA21, SRH20].
Investigating [CPK22, HOVG20b, KMG22]. **Investigation**
 [BB20, JXL⁺21, MKD21, MEWD20, SG20, ZLH⁺20b, AN20, AJC⁺21,
 BTS⁺21, CLS⁺22, CBK⁺20, ER22, GNC20, GSRG22, HBB⁺21, HMBPJ⁺20,
 Kan22, Kid21, LC20, LYTS20, LLMQ20, LLQ⁺21, MOB21, OGSPP⁺22,
 Pan20, RMeH⁺20, Roy20, SCZ21, SBJ20, TT21b, UV20, WZL⁺21, YYL21,
 ZJW⁺21, dPZFM⁺22]. **investigations**
 [KWWZ20, KA21, LYT⁺20, LHL⁺21, LXWZ21, MSKA20, RCM⁺22].
involve [LFMG20]. **involved** [CMM⁺22]. **iodine** [MF21b]. **ion**
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 VdM22]. **ion-pair** [VdM22]. **ionic** [ÉC21, FK20, LNE⁺20, THL⁺21].
ionization [BBG20, MHD20]. **Ionized** [ÜB20]. **ions**
 [BVL22, CLS⁺22, HOVG20b, NZAH21, RED21]. **IOTC** [BCKN21].
IOTC/CASSCF/CASPT2 [BCKN21]. **IQA** [LFMG20]. **IR**
 [SN21, DSNZ⁺20]. **IRC** [QDOC⁺21]. **IRC-Analysis** [QDOC⁺21]. **IRMOF**
 [RDMF21]. **IRMOF-8** [RDMF21]. **iron** [VSKG21]. **irradiation** [LYW⁺20].
iso [TVdVN21, TVdVN22]. **iso-electronic** [TVdVN21, TVdVN22].
isocyanic [ZLT⁺20]. **isolated** [PVR20]. **isomer** [MFC20a, TWT⁺21].
Isomerism [AS22]. **isomerization** [JD20]. **isomers**
 [BWLZ22, WYZZ20, dLRdLJ⁺20]. **isomorphic** [PASS21]. **isoprene**
 [SRS21, TXW⁺20]. **isospectral** [GN21a]. **isotope** [DKK⁺20]. **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,
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 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, HOVG20a, INV22a, KKRR21, MBR21b, MM22b, RBSW21a,

SFT^{+21a}, WV20a, Ano20-47]. **István** [CPK22, SSL22]. **IV** [ASHPHCB20, HLL20a, STF21, VSKG21].

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

Kekulé [RRD⁺²²]. **Kekulé-** [RRD⁺²²]. **Keto** [KMK21, LZS20, SLdS20]. **Keto-enol** [KMK21, LZS20, SLdS20]. **ketones** [LZ21]. **ketoxime** [YYL21]. **key** [SKR⁺²¹]. **kinase** [WV21]. **Kinetic** [BWLZ22, MWC⁺²¹, VdM22, YST⁺²¹]. **kinetically** [KRK⁺²¹]. **Kinetics** [SRS21, KI20, YZD⁺²⁰, ZZZ^{+20a}, ZHS21]. **Kirchhoff** [Ye20]. **knowledge** [Nag20a]. **KOALA** [Höf21]. **KOBu** [VOK⁺²⁰]. **KOH** [VOK⁺²⁰]. **Kr** [dAOdASP⁺²⁰]. **Kratzer** [AIN⁺²⁰, GN21b].

L [RR21, JAZ⁺²⁰]. **L-** [JAZ⁺²⁰]. **L1** [KLT21]. **lab** [Nag20a]. **lactamase** [KLT21]. **LaFe** [MTA⁺²²]. **Lagrangian** [SY21]. **landscape** [RK21]. **landscapes** [Röh21]. **lanthanide** [Kov20, SFPH22]. **lanthanum** [RKG21]. **LaO** [MEWD20]. **lapatinib** [HBY20]. **Laplacian** [LZSA20, LXZ21b]. **Large** [RMLPGHP20, TSW⁺²⁰]. **laser** [Dau21, GZCY22, HSV22]. **laser-dressed** [HSV22]. **lateral** [OGSPP⁺²²]. **lattice** [ACM20, FCL22, LHL⁺²¹, LXWZ21, ZX21]. **lattice-strain** [LXWZ21]. **lattices** [DQS⁺²¹]. **layered** [FMH⁺²², MEWD20]. **layers** [MKKA21]. **LC** [HMN20]. **LC-DFT** [HMN20]. **lead** [MNWD20, PAS⁺²¹, ZZLC20]. **lead-halide** [ZZLC20]. **leading** [MSADA21]. **learning** [FH21, LACP21, RP22, WWLL21, ZX21]. **least** [PJ20b]. **least-squares** [PJ20b]. **length** [ZZ22]. **lepton** [BA22b]. **level** [LNE⁺²⁰, ZLT⁺²⁰, ZYZ^{+21a}, ZYZ^{+21b}]. **levels** [JS21]. **Lewis** [RKG21, SSIE20, WWWC21]. **Li** [Ari21, Yan21, ZXS21, ABDD22, FK20, MHS21, PC22, RS21, RNRBFC21, SBA21, SPR22, TVdVN21, TVdVN22, ZYZ⁺²²]. **Li-decorated** [RS21]. **Li-like** [TVdVN21, TVdVN22]. **Li-metal** [ZYZ⁺²²]. **LiBH** [KHH⁺²¹]. **Libra** [TJA20]. **life** [HYY20]. **ligand** [KKH21, NHNO20, WHYL21]. **ligand-promoted** [WHYL21]. **ligands** [DSNZ⁺²⁰, SCAD⁺²⁰, ZPS⁺²⁰]. **ligated** [DDSB22, Mok21a]. **Light** [KGSD20, BGK⁺²², Fin21, GRZ⁺²¹, LK20, LYW⁺²⁰, WAM⁺²⁰, WZ21]. **light-driven** [WAM⁺²⁰]. **Light-induced** [KGSD20]. **like** [AJC⁺²¹, ARBM21, Ano22a, BT21, CLS⁺²², CBK⁺²⁰, DL21, JVK22, NZAH21, dOSdASC⁺²⁰, SSD22, TVdVN21, TVdVN22, WZ20, XJLH21, dPZFM⁺²²]. **limit** [PMGR⁺²¹, Var21]. **line** [HSV22, LS21]. **Linear** [GXL⁺²², OR21, ZGJ⁺²⁰, AMM21, DS20, GZC21, HP21, LMMA21, PM22, ZMJ⁺²⁰]. **linear-scale** [ZMJ⁺²⁰]. **linked** [DCY21]. **liquids** [LNE⁺²⁰, THL⁺²¹]. **lithium** [FMH⁺²², MZF21, MHS21, dRNS21, RBJ21, Yan21]. **lithium-ion** [MHS21, dRNS21]. **lithium-sulfur** [MZF21]. **Ln** [Kov20]. **Local**

[AIB21, DK21, GTV20, Izs21, Roy20]. **local-density** [GTV20]. **Localization** [GN21b, KRB20]. **localized** [STI20, TWT⁺21]. **logic** [TPT20]. **long** [EB22, KA21]. **long-range** [EB22, KA21]. **longevity** [Nag20a]. **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** [BXWK22, LYTS20, TVdVN22]. **luminescence** [DSNZ⁺20]. **luminescent** [SYL⁺21]. **LuZ** [MBM⁺21]. **lying** [MM21, dLRdLJ⁺20].

M [Ari21, HBB⁺21, HDF⁺21, KS21, LZZ⁺20, OMA21, PZGH⁺20, PCKP20, QOM⁺20, Shi21, Tia21, Yan20, Ari21, LZZ⁺20, OMA21]. **M-N** [KS21]. **Machine** [WWLL21, ZX21, FH21, RP22]. **made** [Mok21b]. **magic** [ELH20, WKH20]. **magnesium** [ZZZ20b]. **Magnetic** [LZS20, sLLqX⁺20, AJC⁺21, CPL⁺21, CLLC21, GGUU21, HOVG20b, HNO⁺21, KA21, LBP20, MBM⁺21, MT21, OAJ21, ONH⁺21, RG20, TMH21, VCM⁺21, Yan21, ZYZ⁺22, ZPS⁺20]. **Magnetically** [PM20]. **magnetism** [DYG21, GOR20, GYC20, PKBZ20]. **Magneto** [BU20, BBAA21, KMG22, SG20]. **magneto-electronic** [BBAA21, KMG22, SG20]. **Magneto-optical** [BU20]. **Magnetoelectronic** [AMK⁺20, BB20]. **Maintaining** [SF20b]. **Majorana** [LMMA21]. **malonic** [SLdS20]. **malonitrile** [BRB⁺21]. **manager** [KS22]. **manipulation** [DRV20]. **Many** [UP20, RKI20, SMJ20, YÇDÖ21]. **Many-body** [UP20, RKI20, SMJ20]. **map** [PJ20b]. **Markovnikov** [LG21]. **material** [KDY⁺22, LFX⁺21, MJRS20]. **materials** [AKK⁺21, CRC21, EGLJQ⁺21, FSR⁺22, JHH⁺22, KMH⁺20, KM21a, LZ20, MZF21, MHS21, RKA⁺21, RINHY20, SCZ21, SUG20, 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]. **maximum** [ADZA21]. **Maxwell** [BRF21]. **Mayer** [CPK22, SSL22]. **MB** [Tia21]. **McDonald** [BXWK22]. **mean** [CFJ20]. **mean-field** [CFJ20]. **means** [BVL22]. **measures** [MSA22, Ole21]. **Measuring** [AD22]. **Mechanical** [JSF⁺21, CMGH⁺21, JZX⁺20, KHH⁺21, Kön21, KMG22, LZZ⁺20, ORL⁺20a, OMA21, PL20, PJ20a, Pan22, PKBZ20, PP21, XFW⁺20, YCL⁺22, ZRR⁺21, ZLH⁺20b]. **Mechanically** [PAS⁺21]. **mechanics** [BRF21, LACP21, NF20, ZMJ⁺20, GPP⁺21]. **mechanics/Gromacs** [GPP⁺21]. **Mechanism** [LZ21, YZD⁺20, ZZZ⁺20a, ZZL⁺20a, ZHS21, BZP⁺20, CSY⁺21, CMM⁺22, ES21, GYC20, HRTSS⁺20, HYC⁺21, JRA21, JXYL20, KI20, LWW20, LZL⁺21, LLQ⁺21, SSEI21, SE20, SRS21, SYL⁺21, SYT⁺21, TXW⁺20, TCX⁺22, TSHRS⁺20, WLP⁺20, WSSD21, YZL⁺21b, YHW⁺22, YHZ⁺22, ZWW⁺22]. **Mechanisms** [SBG21, LLLL20, LFMG20, VOK⁺20, WCZ⁺20]. **Mechanistic** [BTS⁺21, WLH⁺20, WHYL21, AAN⁺21, HW21b, LG21, YST⁺21]. **media** [KAUB21, Üng20]. **mediated** [ER22, PD22]. **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]. **metal**
 [AKKN20, Ari21, ARRB⁺21, BTS⁺21, CYJC20, DTAS21, FK20, HRTSS⁺20,
 JZX⁺20, JXM22, Kan22, KM21a, LL21, NG20, OAJ21, PIA21, Pan20, PC22,
 SCAD⁺20, SRH20, UBW⁺22, VN21, WWM⁺21, XQJ⁺21, YZY⁺22, ZYZ⁺22].
metal-anthracene [YZY⁺22]. **metal-doped** [Pan20]. **metal-free**
 [AKKN20, PIA21]. **metal-nitrogen** [PC22]. **metal-organic** [HRTSS⁺20].
metal-salen [CYJC20]. **metallated** [Üng20]. **metallic**
 [BB20, CYJC20, 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, GRZ⁺21, KM21a, MKKK22, RHS⁺21].
methacrylate [DFK20]. **Methane** [DB20, RSD21, RDMF21, XCZ⁺21].
Method [MMM20, ATL⁺20, Ano22a, BT21, BBG20, Cin20, GM21, KH20,
 LLC20, MMM16, NF20, NLA⁺21, Pon19, Rad21, Rui22, STI20, SY21,
 SYL⁺21, TCSG⁺20, ZHJ⁺20]. **Methods**
 [ZG21, Boz21, CLS⁺22, Eti20, FH21, GZC21, HP21, PPCF⁺20, Pev21,
 Röhh21, SRH20, SS21, WWL21, WP20, ZMJ⁺20]. **methoxyethyl** [YST⁺21].
methyl [CLL20, DFK20, MSM⁺20, SRS21]. **methylidyne** [ASO⁺22].
metronidazole [MJA20]. **Mg**
 [Ari21, PCKP20, Tia21, AAB22, HYC⁺21, KAG⁺20, WWM⁺21]. **MgB**
 [LWH⁺21]. **MgTi** [Kan21]. **MgV** [Kan21]. **MH** [PCKP20]. **microhydration**
 [MHD20]. **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]. **misfolding** [Hol21]. **mitigator** [UBV⁺21]. **MM**
 [CN21, SYL⁺21]. **Mn** [LHL⁺21, MBM⁺21, ONH⁺21, SG20, WWZ⁺21].
Mn-based [SG20]. **Mn-corrolazine** [WWZ⁺21]. **MNg** [Yan20]. **MnGe**
 [TT21b]. **MnO** [MHS21]. **MnX** [GGUU21]. **Mo**
 [OMA21, PP21, PPCF⁺20, PP21]. **mobility** [ZZ22]. **model**
 [AkAR⁺21, ABS20, KGSD20, NSM22, TSN⁺21, TAS21, BVL22]. **Modeling**
 [KMK21, Doh20, Hav21, KI20, LL20, ORL⁺20a, Sta21, TPB⁺20]. **models**
 [FK20, Fin21, VL21, VOK⁺20]. **moderate** [DB20]. **modes** [WZ21, YXKJ21].
modification [HBY20, MSKA20]. **modified** [XCZ⁺21]. **Modulation**
 [LZ20, BSS21]. **moiety** [FFBH21]. **Molecular** [DTW21, FZL⁺20, FAJOF20,
 HTNP21, HLL20a, JXL⁺21, PIA21, RPAA22, RP22, SIA20, SSIE20, WV20b,
 XWLZ20, ZZXT21, Ano22a, BMH21, Boz21, BT21, CZ21, DKK⁺20, GOR20,
 GDR21, Gun21, GZCY22, GM21, IMJ21b, JAZ⁺20, JJJM21, KZ21, MZD⁺20,
 MW21, MNN⁺20, MWC⁺21, MSADA21, NF20, RA20, RKI20, RKG21, RC20,
 SP20a, Shi20, SA20, TCL⁺21, TCX⁺22, TPT20, WWL21, WAM⁺20, WY20,

WP22, YZY⁺²², ZMJ⁺²⁰, ZYZ^{+21a}, ZKP22, MNN⁺²⁰]. **Molecular-scale** [SIA20]. **molecule** [BCKN21, GRLH21, LC20, ÖÇÖ21]. **molecules** [AMM21, BUF⁺²², BCM⁺²², BA22b, CBB21, Doh20, GOS20, HSV22, HTNP21, HJIO21, ID21, JS21, KJA⁺²¹, LZ20, Mok21b, MAMB⁺²², NHNO20, NR21, PNC20, Rad21, RED21, SSIE21, Sta21, TTTH20, WAM⁺²⁰, XJ20, Yan21]. **Molint** [Boz21]. **Møller** [HLL20a]. **molybdate** [HOVG20b]. **molybdenum** [AKK⁺²¹, RK21]. **Moment** [RSBK20, AJC⁺²¹, CZ21, HTNP21]. **moments** [AKP22, BCM⁺²²]. **monoborides** [XQJ⁺²¹]. **monocation** [WAW⁺²¹]. **monoclinic** [Pan22, ZX21]. **monohydroxycinnamic** [BVT20]. **monoketone** [LWR21]. **monolayer** [CLLC21, HZC21, MKKK22, MNWD20, RS21, SPF⁺²², UP20, tZNB⁺²²]. **monolayers** [XHX⁺²⁰]. **mononitride** [sLhZX⁺²²]. **Monosubstituted** [Cha21a]. **monoxide** [THS20]. **Monte** [SRH20, HZC21, NZ20, SS21]. **Monte-Carlo** [SS21]. **MoO** [HOVG20b, WLP⁺²⁰]. **MoPro** [Shi21]. **MoPro-H** [Shi21]. **Morse** [BU20, PMGR⁺²¹, SS21]. **MoS** [UP20]. **Mössbauer** [GKPK21]. **most** [SBM22]. **Mostar** [AIAG21, AII21, DL21, IAI20, MAK⁺²²]. **motion** [BBG20, Dau21, Eti20, FGMO20, Izs21, RRSF22, TJA20]. **motor** [WAM⁺²⁰]. **movement** [BS20]. **Moving** [LLC20]. **MP2** [QdOdMC⁺²¹]. **MRhSb** [HBB⁺²¹]. **MSbO** [PZGH⁺²⁰]. **multi** [ABDD22, JBPV21, MKD21, SZMM22, ZS21, dLRdLJ⁺²⁰]. **multi-configuration** [ZS21]. **multi-Diels** [ABDD22]. **multi-dimensional** [SZMM22]. **multi-reference** [JBPV21, dLRdLJ⁺²⁰]. **Multidimensional** [LLC20, TPCSD20]. **multielectron** [GM21]. **multifunctionalized** [MZ21]. **Multilevel** [HK22, Kön21]. **multinitro** [XWLZ20]. **multinitro-triazole** [XWLZ20]. **multiparameter** [PMGR⁺²¹, XJ20]. **multiphoton** [JWZZ20]. **Multiple** [LYT⁺²⁰, SD20]. **multireference** [dSFdSdMm20, GDR21, JJJM21]. **Multiscale** [Doh20, CN21, ZLH20a]. **multivalent** [KM21a]. **MXene** [LLZC20]. **MXenes** [LZZ⁺²⁰].

N [APR20, EB22, Kov20, KS21, NG20, RINHY20, WWWC21, YCPW20, dPZFM⁺²², Yan21, CPL⁺²¹, ÉC21, JRA21, LFRTRP⁺²⁰, LLMQ20, LXWZ21, MSM⁺²⁰, MSS22, MNWD20, NHNO20, NZ20, RG20, SSIE20, SSEI21, SDL⁺²², SBG21, TCX⁺²², XHX⁺²⁰, XQJ⁺²¹]. **N-containing** [SSEI21]. **N-dopant** [LXWZ21]. **N-doped** [SDL⁺²²]. **N-heterocyclic** [JRA21]. **Na-ion** [LFX⁺²¹]. **Nakatsuji** [Sør21]. **nano** [KAUB21, dPZFM⁺²²]. **nano-cage** [dPZFM⁺²²]. **nano-composites** [KAUB21]. **nanoclusters** [DYG21, ER22, FPdS21]. **nanocomposites** [UBW⁺²²]. **nanocones** [Ali20, Jah20, ZMS21]. **nanocrystal** [FCL22]. **nanohybrids** [Mok21b]. **nanomaterials** [MZ21]. **nanoplastics** [Hol21]. **nanoring** [Mok21b]. **nanosheets** [DJC21]. **nanosize** [DCY21]. **nanostructures** [AII21, IAI20, KOB20, MAK⁺²², ZZLC20]. **nanotori** [Ali20, Jah20]. **nanotube** [KS21, MJA20]. **nanotube-based** [KS21]. **nanotubes**

[AA20, DQS⁺²¹, IMJ21a, IMJ21b, MCP⁺²⁰, NS22, Roy20, SZMM22, THS20].
natural [LFRTRP⁺²⁰, Roy20, SIA20, 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]. **NdCo** [BBAA21]. **NdRu** [KMG22]. **near** [BM21, PZGH⁺²⁰]. **near-equilibrium** [BM21].
nearsightedness [HRA⁺²²]. **necessary** [Sør21]. **negative** [MOB21].
neighboring [BCM⁺²²]. **network** [AkAR⁺²¹, HW21a, WWL21]. **networks** [LPH22, ÖÇÖ21]. **Neumann** [Ole20, Ole21]. **neural** [AkAR⁺²¹, WWL21].
neutral [AN20, ABDD22, FK20, KDY⁺²², KMK21, MZXL21, MFC20a].
newly [SG20]. **Next** [WAM⁺²⁰]. **Next-generation** [WAM⁺²⁰]. **Ng** [dAOdASP⁺²⁰, Yan20]. **NH** [PAS⁺²¹, PLT⁺²⁰, RR21, MSS20, WZL⁺²¹].
NHC [LZ21]. **NHC-catalyzed** [LZ21]. **Ni** [EB22, KYL⁺²⁰, DB20, EB22, RSD21, UBV⁺²¹]. **Ni-W** [UBV⁺²¹]. **nickel** [LG21]. **nickel-catalyzed** [LG21]. **NiI** [MKM⁺²⁰]. **Niko** [Ano22a]. **nitrate** [SK20]. **nitride** [CPL⁺²¹, MCP⁺²⁰]. **nitro** [JXL⁺²¹]. **nitroalkenes** [KZ21].
nitroaromatics [ZKP22]. **nitrogen** [HNO⁺²¹, PC22, SBG21, THS20, WXLL21, ZJW⁺²¹, ZZXT21].
nitrogen-incorporated [HNO⁺²¹]. **nitrogen-rich** [ZJW⁺²¹]. **nitroso** [HBY20, YCSK20]. **nitrosyl** [RR21]. **nitrotriazoles** [XWJ⁺²¹]. **Nix** [KS22].
NMR [CRKMC21, GZC21, GMRKMCMC21, HMN20, SSK20, SK21].
NMR-shielding [CRKMC21]. **NO** [RR21, YST⁺²¹, Kid21, MZ21, WZL⁺²¹, ZZLY22]. **noble** [AN20, dAOdASP⁺²⁰, TTTH20]. **noble-gas-containing** [TTTH20]. **Non** [CMM21, BA22a, GXL⁺²², LMA21, MC22, MM21, NG20, RKA⁺²¹, XAM⁺²², SPR22]. **Non-adiabatic** [CMM21, MM21]. **non-central** [BA22a]. **non-covalent** [MC22]. **non-fullerene** [GXL⁺²²]. **non-Hermitian** [LMA21]. **non-metal** [NG20]. **Non-relativistic** [SPR22]. **non-scalar** [XAM⁺²²]. **non-toxic** [RKA⁺²¹]. **nonadiabatic** [MKD21]. **nonadjacently** [ZMS21]. **noncentral** [GN20]. **Noncovalent** [ZKP22, OGT20, TCSG⁺²⁰]. **nondoped** [SYL⁺²¹]. **nonelectrostatic** [VL21]. **Nonempirical** [HMBPJ⁺²⁰].
nonideal [DG21]. **Nonlinear** [BMF20, BRB⁺²¹, GXL⁺²², HDF⁺²¹, LYT⁺²⁰, SFB20, TSW⁺²⁰, ZXS21].
nonlocal [Hua20]. **nonmetallic** [LK21]. **nonpolar** [LLZ⁺²⁰].
nonrelativistic [SPR21]. **NOO** [YCSK20]. **Normal** [Bra21]. **normalized** [LZSA20]. **norms** [SSD22]. **novel** [FZL⁺²⁰, HBB⁺²¹, Hav21, TSW⁺²⁰, WJL⁺²¹, ZLH20a, ZLH^{+20b}]. **Nuclear** [DKK⁺²⁰, FGMO20, OAJ21, RKI20, RRSF22, SSIE20, VCM⁺²¹]. **nuclei** [OAJ21]. **nucleobase** [UAH⁺²⁰]. **nucleon** [GRFM20]. **nucleophiles** [LWC⁺²¹]. **number** [CDR20, ELH20, HDF⁺²¹]. **Numerical** [SS21].

O [FK20, GNC20, JXYL20, JZL⁺²¹, Kan21, LZL⁺²¹, MKD21, MTA⁺²², 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}].

obtained [YZY⁺21b]. occupied [ATL⁺20]. octafluoro [GB21, YHW⁺22]. **Octafluoro-2-butene** [YHW⁺22]. **octafluoro-spirobi** [GB21]. **octane** [WYZZ20]. **odd** [WZ20]. **off** [Cio22]. **off-diagonal** [Cio22]. **OH** [HYC⁺21, YST⁺21, MOB21, YZD⁺20]. **OH-bonded** [MOB21]. **OH-initiated** [YZD⁺20]. **oils** [AAN⁺21]. **OLED** [SCZ21]. **OLEDs** [LYTS20]. **oligomer** [WZ20]. **oligomer-like** [WZ20]. **oligomers** [MWBQ20, OR21]. **oligophenylenes** [INV22b]. **oligothiophene** [ZZ22]. **OM** [HDF⁺21]. **One** [LBG20, Cio22, Eti20, JXL⁺21, LFMG20, Ole20, PMGR⁺21, WCZ⁺20, ZYZ⁺22]. **one-body** [Eti20]. **one-dimensional** [Ole20, PMGR⁺21, ZYZ⁺22]. **one-electron** [Cio22]. **one-step** [LFMG20, WCZ⁺20]. **ONIOM** [THS20]. **open** [MJRS20, SF20a, HHG⁺21]. **opening** [CYJC20, dSFdSdMdM20, MAMB⁺22]. **operations** [AIAG21, AD22, IAI20]. **operator** [Yos20]. **opposite** [WXLL21]. **Optical** [BUKA21, INV22b, KB21, Mok21a, BU20, BRB⁺21, GXL⁺22, GGUU21, HNO⁺21, HDF⁺21, LLZC20, LYT⁺20, MKuAS⁺22, MAHRA⁺21, MRI20, MIM21, MTA⁺22, Pan20, SFB20, TSW⁺20, Üng20, WV21, ZZLC20, 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** [AAB22, AAM⁺20, HBB⁺21, KHH⁺21, ZRR⁺21]. **optomechanical** [BGK⁺22]. **orbit** [AAM⁺20, Iri20, Iri21, KWWZ20, ZS21]. **Orbital** [MMM20, Cin20, LFRTRP⁺20, MBKA21, MMM16, Nag20b, NF20, Roy20, SP20a, TPB⁺20, GSMT⁺20]. **orbital-free** [Nag20b]. **Orbital-Specific** [MMM20, Cin20, MMM16]. **orbitals** [GM21, LFRTRP⁺20, Lom21, SM22, Sha20, SA20]. **orbits** [JVK22]. **Order** [ACM20, ATL⁺20, ADZA21, Cio22, GXL⁺22, HDF⁺21, sLLqX⁺20, PM22, SM22]. **Ordering** [LYFL21]. **orders** [CPK22]. **organic** [BZW⁺20, BSS21, BRB⁺21, FZL⁺20, HRTSS⁺20, HW21a, ID21, KMH⁺20, KJA⁺21, LK20, MSKA20, MSKA21, MKuAS⁺22, NIA21, NLA⁺21, PIA21, PGPHAPM20, PVR20, PD22, PC22, PNC20, TSW⁺20, ZGCF20]. **organization** [RKG21]. **organocatalysts** [SSIE21]. **organocatalytic** [LLQ⁺21]. **organosilicon** [HCZ20]. **orientation** [GZCY22]. **Orientations** [BMR21]. **Oriented** [WWZ⁺21, ZYZ⁺21a]. **origin** [HYY20]. **origins** [GA20]. **ORR** [KS21]. **ortho** [WLH⁺20, YCSK20]. **ortho-selective** [WLH⁺20]. **oscillator** [GN21a, HJIO21, OB21b, WWKH22, YÇDÖ21, TdV21]. **OTf** [TXW⁺20]. **outstanding** [XWLZ20]. **overlap** [GM21]. **oxidation** [CLC⁺21, ER22, SKR⁺21, VGSS20, WXLL21, WWZ⁺21, YST⁺21]. **oxidative** [ZZZW20]. **oxide** [BTS⁺21, CYJC20, IMJ21a, IMJ21b, KBR⁺20, KM21a, MI20, MSADA21, MNWD20, VN21, ZHFD⁺20]. **oxides** [KKH21, Kan22, ORL⁺20a, XWJ⁺21, YCSK20]. **oximes** [DDSB22]. **oxoiron** [VGSS20]. **oxyethoxy** [ZWL22]. **oxygen** [DB20, GKPK21, JJJM21, PZGH⁺20, TCL⁺21, VKS21, XWLZ20, ZHFD⁺20]. **oxyl** [SKR⁺21]. **oxypnictides** [MEWD20]. **ozonolysis** [LWW20].

P [LFRTRP⁺20, MEWD20, GZC21, RINHY20, WSSD21]. **P-doped** [RINHY20]. **package** [KS22, TJA20]. **packaging** [KS22]. **packet** [Dau21]. **pair** [MHD20, Roy20, VdM22]. **pairs** [SSIE20]. **palladium** [STI20]. **para** [LS21, INV22b]. **para-line** [LS21]. **para}-oligophenylenes** [INV22b]. **paradigm** [RPT21b]. **paradigms** [Mos21]. **Parallel** [GNC20]. **parameter** [NLA⁺21, RPT21a, SSD22]. **Parameterization** [PPR21]. **parameters** [FSR⁺22, KJA⁺21, Pev21, RRD⁺22, RPT21b, TCSG⁺20, ZX21]. **paraquat** [HW21b]. **part** [JJJM21]. **partial** [JBPV21]. **Particle** [LRG⁺20, AJC⁺21, GRFM20, LMA21]. **Partitioning** [CBB21]. **Path** [DKK⁺20, BM21, CMY22, LYTS20]. **pathways** [BZW⁺21, SFPH22, WZL⁺21]. **patients** [KAA21]. **pattern** [DYG21]. **patterns** [CRKMC21, GMRKMC21]. **Pauli** [Sah21]. **Pb** [Shi21, XFW⁺20, KDY⁺22]. **PbX** [PAS⁺21]. **Pd** [QOM⁺20, SDL⁺22]. **PdZn** [LSS⁺21]. **penalty** [KH20]. **penta** [LZSA20]. **penta-graphene** [LZSA20]. **pentagonal** [ZMS21]. **pentamer** [MC22, XBK⁺20]. **pentane** [LZS20]. **pentane-2** [LZS20]. **pentanitrogen** [Mka20]. **pentothal** [CDG⁺21].

Performance [MZ21, AAB22, AKKN20, BSS21, EGLJQ⁺21, FFBH21, HMN20, LK20, LL20, MHS21, NIA21, NLA⁺21, SUG20, WLY⁺20, WWZ⁺20, YZL21a, YCL⁺22].

performances [LXZ⁺21a, SSIE21, VL21]. **perhalogenated** [SC21]. **periodic** [PGPHAPM20]. **periodically** [KRB20]. **peripherality** [AD22]. **perovskite** [AAM⁺20, BPB⁺20, LZ20, RMeH⁺20, ZZLC20, ZCL⁺22]. **perovskite-type** [RMeH⁺20]. **perovskites** [NG20, PAS⁺21, ZX21]. **peroxidase** [KI20]. **peroxide** [CSY⁺21]. **perspective** [AKP22, GG20a, GG22, KZ21, KMG22, OGT20, PM20, RS21, SIA20, TAS21, XAM⁺22]. **perspectives** [EPMC20, PAS⁺21, Sah21]. **perturbation** [AIB21, BMF20, HLL20a, SM22, ZIA20]. **phase** [CRC21, CSK21, Dau21, DPC⁺20, GOS20, GRLH21, HLL20a, LZL⁺21, ORL⁺20b, RMLPGHP20, RKI20, SDS19, SDS20, SASA21, Shi21, SG21, VdM22]. **phase-dependent** [Dau21]. **phases** [ARRB⁺21]. **phenol** [YST⁺21]. **Phenyl** [ZXS20]. **phenylene** [FYL21, LZS20]. **phonon** [PKBZ20]. **phores** [LYT⁺20]. **phosphonic** [FFBH21]. **phosphorene** [GG20a, THL⁺21, WLY⁺20, ZHFD⁺20]. **phosphorus** [RBJ21]. **phosphorus-doped** [RBJ21]. **phosphorylcholine** [RYC⁺20]. **photo** [TSN⁺21]. **photo-detachment** [TSN⁺21]. **photoassociation** [JWZZ20, Wan21]. **photocatalyst** [RINHY20]. **photocatalytic** [DLZ⁺21, LYW⁺20, RHS⁺21, WLY⁺20]. **photochemical** [CMM21]. **photoelectron** [GYC20]. **photoelectronic** [XHX⁺20]. **photoinjection** [MSKA21]. **photon** [BMF20, GA20, LXZ⁺21a, SIA21]. **Photophysical** [SFPH22, YLL⁺20, ZLH20a]. **photosensitizers** [MSKA20, SIA20]. **Photovoltaic** [SIA20, BZW⁺20, BSS21, FFBH21, FSR⁺22, GSRG22, JHH⁺22, KMH⁺20, KJA⁺21, XPZ20]. **phthalocyanines** [MSA22]. **physical** [RCM⁺22, RKA⁺21]. **physico** [RNB22]. **physico-chemical** [RNB22]. **picture** [JVK22]. **piezoelectric** [MT21]. **place** [CLS⁺22]. **Planar**

[ZFB⁺20, APR20, KRK⁺21, TT21a]. **plane** [MM20, STI20]. **plasma** [Bah22, BMF20, CLS⁺22, KB21]. **plasmas** [DG21]. **plasmon** [UBW⁺22, KAUB21]. **Plasmonic** [Mok21b]. **Platinum** [PD22, Iri20, Iri21]. **Plesset** [HLL20a]. **plutonium** [RED21]. **Pn** [MEWD20]. **pnicoen** [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, JS21, WP22, YÇDÖ21]. **polarizability** [CBB21]. **Polarizable** [BVL22]. **polarization** [PM22, STT20, WP22]. **polarizing** [MT21]. **pollutants** [ARBM21]. **polyacene** [KA21]. **polyatomic** [BUF⁺22]. **polychromatic** [TSN⁺21]. **polycyclic** [Rad21]. **polymer** [MW21]. **polymerization** [DYK22]. **polynitrocubane** [LL20]. **polynomials** [SSD22]. **polyoxometalates** [CSY⁺21]. **polyoxometalates-supported** [CSY⁺21]. **polyphenyls** [DL21]. **polytypes** [ORL⁺20b]. **POMzites** [VN21]. **Pons** [Yos20]. **population** [DC22, MKD21]. **pore** [HDF⁺21]. **porphyrazines** [BWBR21]. **porphyrin** [GMO⁺20, Üng20, WFG⁺21]. **porphyrin-** [GMO⁺20]. **porphyrins** [MSA22, Üng20]. **Pöschl** [HJIO21, PMdN21]. **position** [BS20, SSIE20]. **positive** [MOB21]. **positron** [BA22a, STT20]. **positron-electron** [STT20]. **possible** [AMK⁺20, Yan20]. **Post** [Var21]. **Post-complete-basis-set** [Var21]. **potassium** [HJIO21]. **Potential** [MC22, MMM20, RK21, ABS20, AIN⁺20, AB21, BUKA21, BBG20, Dau21, EGLJQ⁺21, FSR⁺22, GN20, GN21b, GG20b, HLL20b, IRA⁺20, JBPV21, KDY⁺22, Kid21, KH20, LFX⁺21, MSS20, NACP21, NR21, Nat22, OO21a, OO21b, PMGR⁺21, PMdN21, PJ20b, RS21, RKI20, RR21, SSIE20, SFPH22, SS21, SKG21, STT20, TCL⁺21, XJ20, ZGCF20, MM22a]. **potential-based** [JBPV21]. **potentials** [BA22a, BAM20, Cin20, DFB20, EB22, GN21a, MF21a, MMM16, MZT20, PGROM20, PJ20b, WWKH22, XJLH21, ZYZ⁺22]. **Povarov** [LLQ⁺21]. **powder** [FCL22, HYC⁺21]. **PPh** [QOM⁺20]. **practical** [Pon19]. **prebiotic** [ES21, SE20]. **precision** [XJLH21]. **predicted** [WJF⁺21]. **Prediction** [ARRB⁺21, BVL22, HW21a, PP21, Rac21, GZC21, MRI20, WWL21, WWLL21, Yan21]. **predictions** [GZC21, SKR⁺21, SBG21]. **predictor** [SJ20]. **predominately** [SF20b]. **preference** [FCL22]. **Preliminary** [KRS⁺21]. **prenucleation** [SP20a]. **preorganized** [ÖÇÖ21]. **preparation** [AKP22]. **presence** [GN20, GN21b, Hol21, YST⁺21, ZIA20]. **Pressure** [ONH⁺21, YCL⁺22, JSF⁺21, LWH⁺21, MT21, PJ20a, PKBZ20, Sta21, XFW⁺20]. **Pressure-induced** [YCL⁺22]. **pressures** [HLL20a, JZX⁺20, WJF⁺21]. **prevention** [LS21]. **primary** [WDS⁺20]. **principle** [HRA⁺22, KA21, KS21, MHS21, MBM⁺21, RMeH⁺20, UV20, WXL⁺21, XFW⁺20, ZYZ⁺21b]. **principles** [AJC⁺21, AKKN20, DLZ⁺21, ER22, FMH⁺22, GSRG22, GGUU21, JZX⁺20, Kan21, Kan22, KHH⁺21, KMG22, sLLqX⁺20, LHL⁺21, LWH⁺21, LXWZ21, MBKA21, MSKA21, MAHRA⁺21, MNWD20, OGSP⁺22, Pan20, PL20, RS21, RED21, SFT⁺21b, SG21, WWM⁺21, XCZ⁺21, YZL⁺21b, ZRR⁺21, ZLH⁺20b, tZnB⁺22]. **pro**

[PGPHAPM20]. **pro-aromatic** [PGPHAPM20]. **probability** [CSS+21].
probe [BVL22, ZLH20a]. **probes** [LXZ+21a, MF21b]. **Probing** [VM20].
problems [LACP21]. **process** [CLC+21, FCL22, SCZ21]. **processed**
[Bah22, KB21]. **processes** [LRG+20]. **procyanidin** [MWBQ20]. **produce**
[LWC+21]. **produced** [ZWW+22]. **product** [Hao21]. **production**
[MSS20, SRH20]. **productivity** [SF20b]. **products** [MM22c, SYT+21].
professors [BHH20]. **program** [Höf21]. **Projected** [Rui22]. **projection**
[Pon19, Yos20]. **projector** [MM22c]. **Promising**
[LZ20, KMH+20, WJL+21, XHX+20, YHW+22]. **promoted**
[VOK+20, WHYL21, ZZLY22]. **Promoting** [LSS+21, YZD+21]. **promotion**
[DRV20]. **propagator** [GRFM20, PM22]. **propargylic** [LLLL20].
propensity [BVT20]. **properties**
[AMK+20, AAM+20, BA22a, BPB+20, BBAA21, BMF20, BB20, CLS+22,
CMGH+21, CLLC21, DDSB22, DJC21, DCY21, FCL22, GXL+22, GA20,
GRZ+21, GGUU21, HOVG20b, HNO+21, INV22b, JZX+20, JZL+21,
KHH+21, KMH+20, KYL+20, KSP20, KLK21, KMG22, LLZC20, sLhZX+22,
LMA21, LMMA21, LHL+21, LWH+21, LZZ+20, MJA20, MZXL21, MKKA21,
MKKK22, MKuAS+22, MAHRA+21, MRI20, MKM+20, Mok21b, MIM21,
MBM+21, MEWD20, NG20, NR21, NLA+21, ORL+20a, ONH+21, OMA21,
Pan20, PL20, PJ20a, Pan22, PASS21, PKBZ20, PLT+20, PP21, RCM+22,
RRS21, RKA+21, RNB22, RR21, SIA20, STI20, SFPH22, Sha20,
dOSdASC+20, SSD22, SG20, SG21, TMH21, UV20, Üng20, WXL+21,
WJF+21, XPZ20, XFW+20, XCZ+21, XWS+22, YLL+20, YCPW20, ZZY+22,
YFX+22, ZRR+21, ZLH20a, ZWL22, ZLH+20b, ZZZ20b, ZHFD+20, tZNB+22].
property [RNA22, RNB22, ZXS21]. **propylene**
[CYJC20, CSY+21, WLP+20]. **protected** [QOM+20]. **protein**
[GA20, Hol21]. **proton** [JD20]. **protonated** [MZXL21]. **pseudoharmonic**
[GN21a]. **Pseudopotential** [PNC20]. **Pseudopotential-fragment** [PNC20].
pseudospectral [ZHJ+20]. **Pt** [Iri20, Iri21, QOM+20, RCM+22, Shi21,
DLZ+21, MJA20, PPR21, QDC+22, SRH20]. **Pt-decorated** [MJA20]. **Pu**
[sLLqX+20]. **puckered** [tZNB+22]. **pulses** [Dau21, GZCY22]. **pure**
[JZX+20, XWS+22]. **purely** [MOB21]. **purine** [SE20]. **PVDF** [SK20].
PVDF-HFP [SK20]. **PVDF-TrFE** [SK20]. **pyrazine** [PGPHAPM20].
pyridine [WXLL21]. **pyrimidine** [YLL+20]. **pyrrole** [PVR20, SCU21].
pyrroline [MSADA21]. **pysisyphus** [SKG21]. **Python** [ABS20, GPP+21].
Python-based [GPP+21].

QM [CN21, SYL+21]. **QM/MM** [CN21, SYL+21]. **QSAR** [KAA21]. **QSPR**
[Hav21, KLT21, KAA21]. **QSPR/QSAR** [KAA21]. **QTAIM** [LFMG20].
QTAIM/IQA [LFMG20]. **Quantitative** [JPSC20, RNA22, RNB22].
Quantum [BM21, CSK21, GB21, GM21, MJA20, MJRS20, NZ20, ORL+20a,
RBSW21b, SBM22, SD20, Sta21, VOK+20, WP20, AkAR+21, AKP22, BU20,
BUKA21, Bah22, BMF20, BRF21, CM21, Cio22, CLLC21, DKK+20, Dau21,
GG20a, GN21a, GPP+21, GDR21, HHG+21, HCZ20, HZC21, IRA+20, KB21,

Kön21, KS22, LACP21, LC20, LRG⁺20, LLC20, MM22c, MFK22, Mok21a, MAMB⁺22, MIM21, Mos21, NHNO20, Nat22, Ole20, Ole21, OMA21, RMM⁺22, RKI20, SDS19, SDS20, SI20, Sha20, SUG20, Sur20, Sur22, VKS21, WWL21, WAM⁺20, XWS⁺22, ZMJ⁺20, SRH20]. **Quantum-chemical** [GB21, SBM22, VOK⁺20]. **Quantum-classical** [BM21]. **Quantum-phase** [CSK21]. **quartic** [OB21b, TdV21]. **quaternary** [Rac21, WWLL21]. **quaterthiophene** [SV21]. **quest** [Var21].

R [YCSK20]. **Radial** [ZHJ⁺20, PMGR⁺21]. **radiated** [SBG21]. **radiation** [JAZ⁺20]. **Radiative** [TSHRS⁺20]. **radical** [ASO⁺22, BVT20, DYK22, SRS21, SYT⁺21, YST⁺21]. **radical-scavenging** [BVT20]. **radicals** [CLW21, DFK20, DYK22, JAZ⁺20, SCZ21]. **radii** [LYFL21]. **Raman** [FPdS21]. **Randić** [BMR21]. **random** [FYL21, LSG21]. **range** [EB22, KA21, PT21]. **Rank** [CL21]. **Rao** [EAPCD21]. **Rapid** [ÖÇÖ21]. **rare** [MBKA21, NG20]. **rare-earth-based** [NG20]. **rate** [CZW21]. **rates** [BM21]. **ratio** [Nat22]. **ray** [BWBR21, HP21, RG20]. **Rb** [RMeH⁺20, AMK⁺20, GSRG22]. **RDX** [MWC⁺21]. **Re** [KWWZ20, PJ20a]. **reaction** [ASO⁺22, BZP⁺20, BM21, BTS⁺21, CMY22, CSY⁺21, CMM⁺22, dSFdSdMm20, GKPK21, HW21b, JWZZ20, JD20, KZ21, KWWZ20, TCL⁺21, VKS21, VKK⁺21, WY20, WZL⁺21, WWZ⁺21, WCZ⁺20, YYL21, ZZZ⁺20a, ZHS21]. **Reactions** [DFK20, ABDD22, CMM21, CBK⁺20, ES21, HCZ20, LLQ⁺21, MSADA21, MAMB⁺22, QdOdMC⁺21, RRSF22, SBM22, SE20, TPB⁺20, UAH⁺20, VOK⁺20]. **reactive** [HBY20]. **Reactivity** [DYK22, CMM⁺22, KLT21, LWC⁺21, LLMQ20]. **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]. **redox** [HW21b, ZYZ⁺22]. **Reduced** [DS20, ATL⁺20, BMH21, Cio22]. **reduction** [EB22, GKPK21, LXWZ21, MSM⁺20, RR21, SSIE20, VKS21, XQJ⁺21]. **reference** [Eti20, JBPV21, MKD21, dLRdLJ⁺20]. **reforming** [RSD21]. **Regio** [MF21b]. **region** [WZ21]. **regioselective** [WSSD21]. **regression** [GZC21]. **regular** [DQS⁺21]. **Regulating** [GRZ⁺21, WWZ⁺21]. **reinvestigation** [LWW20]. **related** [IMJ21b]. **Relating** [RRD⁺22]. **relation** [LZS20]. **relations** [GM21, JMOW20]. **relationship** [CMM⁺22, JPSC20, RNA22, RNB22, YCSK20]. **Relative** [Nag20b]. **Relativistic** [AKK⁺21, AMM21, JVK22, OAJ21, HOVG20b, HTNP21, KSP20, MSS22, MZT20, OGT20, PT21, QOM⁺20, SPR22, XJLH21]. **relaxation** [CZW21, INV22b]. **release** [Roy20]. **relevant** [HBY20]. **reliable** [KLT21]. **remarkable** [XHX⁺20]. **Remarks** [Ali20]. **Remdesivir** [LS21]. **removal** [FAJOF20]. **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].

reproducible [GKK21]. **repurposed** [LAAP21]. **research** [BHH20, Nag20a, SF20b, Shi20]. **resistance** [NYX⁺21]. **Resonance** [JBPV21, OAJ21]. **resonances** [BAM20]. **resonant** [WZ21]. **Response** [OB21a, AMM21, Bah22, BMF20, DS20, GRZ⁺21, HP21, HDF⁺21, KB21, LZS20, OR21, PM22, Rac21, STN20, UP20, ZZLC20]. **responses** [TSW⁺20]. **responsivity** [YXKJ21]. **REST** [HHG⁺21]. **restrained** [ABS20]. **restricted** [GSMT⁺20]. **retrochalcones** [MK21]. **reveal** [Cio22]. **revealed** [AKKN20]. **Reverse** [Cio22, LYTS20]. **Review** [BRB⁺21, EM21, YST⁺21, AB21, Doh20, LRG⁺20, MP20, RMM⁺22, SBM22]. **revisited** [BCKN21, CMY22, Sør21]. **Revisiting** [APR20, ZHJ⁺20]. **Rh** [GGUU21, 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, MW21, MAMB⁺22, PM20, Tia21, YLL⁺20, ZFB⁺20, ZZL⁺20a]. **ring-opening** [dSFdSdMdM20, 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, MFK22, PGPHPM20]. **ronidazole** [CXZ⁺21]. **roots** [BXWK22]. **Rosen** [BU20]. **rotary** [WAM⁺20]. **rotating** [SS21]. **Rotation** [HJIO21]. **rotational** [WY20, Wan21]. **rotational-excited** [WY20]. **rotaxane** [BS20]. **rotor** [CWY⁺20]. **route** [CLW21, Kön21, MSS20]. **rovibronic** [HSV22]. **row** [JXM22, RNFMC20]. **RPA** [JS21]. **Ru** [RCM⁺22, RR21, BB20, PJ20a]. **rules** [AS22]. **RuPtSb** [RCM⁺22]. **ruthenium** [Kid21, RR21, SCAD⁺20]. **rutile** [DK21].

S [EGLJQ⁺21, EB22, PASS21, PPCF⁺20, SPF⁺22, WAM⁺20, ZFB⁺20, NYX⁺21, dAOdASP⁺20, SK21, SPR21, SPR22, WAM⁺20]. **saddle** [BXWK22]. **Salen** [UBV⁺21, CYJC20, RR21]. **salt** [Yan20]. **salts** [HDF⁺21]. **same** [Rui22]. **sandwich** [DLZ⁺21, KDY⁺22, YZY⁺22]. **Sb** [BB20, KMG22, MEWD20, Yan20, EGLJQ⁺21]. **scalar** [KSP20, XAM⁺22]. **scale** [SIA20, UBV⁺21, ZMJ⁺20]. **Scandium** [CMGH⁺21]. **scattering** [BA22a, BA22b, MSS22, SDK⁺21]. **scavenging** [BVT20]. **SCF** [JXM22]. **scheme** [LFRTRP⁺20, VKK⁺21]. **Schiff** [GG20b]. **Schrodinger** [SS21, HRA⁺22, LBP20, Sah21, SD20]. **Science** [GG22, MNN⁺20]. **Sciences** [MNN⁺20]. **ScK** [AJC⁺21]. **screened** [AIN⁺20, MF21a, SDS19, SDS20, WKH20, WWKH22, XJLH21]. **screened-hydrogenlike** [WKH20]. **screening** [JXL⁺21, dOSdASC⁺20, WJL⁺21, ZJW⁺21]. **screw** [BU20]. **ScYH** [WJF⁺21]. **Se** [EB22, PASS21, SPF⁺22]. **search** [KRK⁺21, KYL⁺20, KAG⁺20, ZFB⁺20]. **second** [ATL⁺20, ADZA21, GXL⁺22, HDF⁺21, NF20, RNFMC20, SM22]. **second-order** [ATL⁺20, GXL⁺22, HDF⁺21, SM22]. **secondary** [AS22].

sections [MW21]. **segregation** [WWM⁺21]. **Selected** [SSK20]. **Selective** [SRH20, HRTSS⁺20, LSS⁺21, MW21, STF21, WLH⁺20]. **selectivity** [GG20a, JRA21, LZ21]. **selenide** [AAB22]. **selenium** [RMLPGHP20]. **Self** [ES21, SE20, SLdS20, Eti20, HK22, HP21, SM22]. **Self-catalytic** [ES21, SE20]. **Self-catalyzed** [SLdS20]. **self-consistent** [HK22, HP21, SM22]. **self-contained** [Eti20]. **semiclassical** [ZHS21]. **semiconducting** [Mok21a, NIA21]. **semiconductor** [DCY21]. **semiempirical** [WWL21]. **Sensing** [HRTSS⁺20, LXZ⁺21a, MJA20, THS20, TSHRS⁺20, dPZFM⁺22]. **sensitivity** [GG20a]. **sensitization** [GG20b]. **sensitized** [FFBH21, FZL⁺20, MSKA20, PIA21, PGPHAPM20]. **sensor** [GG20a]. **separation** [MJRS20]. **sequence** [LLZ⁺20, TVdVN22]. **sequences** [TVdVN21, TVdVN22]. **sequestration** [QdOdMC⁺21]. **series** [AkAR⁺21, GZWL22, JXL⁺21, MAMB⁺22, WZ20, ZPS⁺20]. **SeS** [tZnNb⁺22]. **set** [Cha21b, DK21, HMBPJ⁺20, QdOdMC⁺21, STI20, SM22, SK21, Var21]. **sets** [GSMT⁺20, NLA⁺21, RPT21a, VP20]. **setting** [RPT21a]. **sexipyridine** [ZXS21]. **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]. **shielding** [CRKMC21, HMN20, OAJ21]. **shieldings** [VCM⁺21]. **shift** [GZC21, GMRKCMC21, HMN20]. **Shifts** [Cha21a, SK21]. **Short** [PT21, DYK22]. **Short-range** [PT21]. **Should** [RBSW21b]. **show** [PZGH⁺20]. **Si** [GZWL22, KDY⁺22, VKS21, tZnNb⁺22]. **Si-doped** [VKS21]. **SiB** [PP21]. **SiC** [LFX⁺21]. **side** [LC20]. **significant** [PZGH⁺20]. **signless** [LXZ21b]. **silanes** [SC21]. **silanol** [CSY⁺21]. **silanol-functionalized** [CSY⁺21]. **silica** [UBW⁺22]. **silicene** [Mok21c]. **silicide** [GZWL22]. **silico** [JPSC20, KRK⁺21]. **silicon** [DYG21, FMH⁺22, GYC20, KRK⁺21, MKKK22, ZZZ20b]. **silol** [XPZ20]. **silver** [UBW⁺22]. **SiMg** [ZZZ20b]. **similar** [Hao21]. **similarity** [GN21a, Izs21]. **Simon** [Ano22a]. **simple** [ACM20, THS20, WZ20, ZWW⁺22]. **Simplified** [GSMT⁺20]. **simulated** [TSN⁺21]. **Simulating** [HP21]. **simulation** [DFB20, JAZ⁺20, MWC⁺21, TCX⁺22]. **simulations** [DKK⁺20, Doh20, MZD⁺20]. **Simultaneous** [MOB21, LFMG20]. **sine** [SS21]. **Single** [GM21, VKS21, DLZ⁺21, Eti20]. **single-atom** [DLZ⁺21]. **Single-Center** [GM21]. **single-reference** [Eti20]. **singles** [BBG20, dSFdSdMdM20]. **singlet** [CPK22, JJJM21, LYTS20, TVdVN22]. **singlet-state** [CPK22]. **singly** [KKH21]. **SiO** [WLP⁺20, AII21, MAK⁺22]. **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, NZ20]. **Slater-Type** [GM21]. **Slow** [BGK⁺22]. **small** [AMM21, GW21, KJA⁺21, LAKJ20, ÖÇÖ21]. **small-molecule** [ÖÇÖ21]. **small-sized** [GW21]. **smallest** [ZFB⁺20]. **SmFeO** [MT21]. **SOA** [RKA⁺21]. **sodium** [CDG⁺21, EGLJQ⁺21].

sodium-ion [EGLJQ⁺21]. **soft** [BA22b]. **Software** [MNN⁺20, KS22, TJA20]. **solar** [BSS21, FFBH21, FZL⁺20, JHH⁺22, KMH⁺20, KJA⁺21, LZ20, MSA20, PIA21, PGPAPM20, SIA20]. **solar-cells** [PGPAPM20]. **solid** [CZ21, HLL20a, SBG21]. **solitons** [PMdN21]. **sols** [LLW⁺21]. **solution** [Doh20, HW21b, KMK21, KK21, KLK21, SS21]. **solutions** [CWY⁺20, GN20, PGROM20, RED21, WV21]. **Solvation** [MHD20, RR21]. **Solvent** [HW21b, HOVG20b, MSM⁺20, OAJ21, QdOdMC⁺21, TPT20]. **Solvent-dependent** [HW21b]. **solvents** [MKuAS⁺22, ZYZ⁺22, ZGCF20]. **Sombor** [DTW21, FYL21, LCX⁺21]. **some** [AN20, AIAG21, FYL21, dSFdSdM20, GSMT⁺20, Hao21, Hav21, KAA21, LC20, MK21, MP20]. **SOPPA** [JS21]. **sound** [YFX⁺22]. **space** [ATL⁺20, CN21, HP21, JBPV21, MBR21a]. **spaces** [KRB20, WFG⁺21]. **Spatial** [RPT21b, ZZ22]. **Spatially** [GSMT⁺20, MR21]. **Special** [Ano20-47, KKRR21, WZ21]. **species** [Bra21, KRK⁺21, MM21]. **Specific** [MMM20, Cin20, MMM16]. **specifications** [BU20]. **spectra** [BWBR21, HP21, Kön21, LNE⁺20, RRSF22, SSK20, SN21]. **spectral** [BRB⁺21, CLS⁺22, LYFL21, UP20, ZZZ20b]. **spectroscopy** [FPdS21, GKPK21, GNC20, GYC20, dAOdASP⁺20, PNC20, RYC⁺20]. **spectrum** [GN20, HJIO21, INV22b, JD20, KK21, KLK21, MFC20b, STT20]. **sphere** [MR21]. **spherical** [YÇDÖ21]. **spin** [AAM⁺20, CSK21, CM21, Iri20, Iri21, KWWZ20, KGSD20, Pon19, RR21, SY21, TWT⁺21, TPB⁺20, TVdVN22, VGSS20, Yos20, ZS21, TVdVN22]. **spin-adiabatic** [TPB⁺20]. **spin-coupled** [SY21]. **spin-crossing** [TPB⁺20]. **spin-orbit** [ZS21]. **Spin-singlet** [TVdVN22]. **spin-state** [KGSD20]. **spin-triplet** [TVdVN22]. **spinel** [ORL⁺20a]. **spinterface** [MKM⁺20]. **spintronic** [AMK⁺20, MTA⁺22, TMH21]. **spintronics** [Rac21]. **spirobi** [GB21]. **spirobifullerene** [KMH⁺20]. **Splitting** [DTAS21, LYW⁺20, SSIE20, ZHJ⁺20]. **squares** [PJ20b]. **Sr** [PZGH⁺20, Tia21, XFW⁺20, PZGH⁺20, VCM⁺21]. **SrO** [FPdS21]. **stabilities** [XHX⁺20, ZRR⁺21]. **Stability** [DG21, AN20, BSS21, DYG21, FPdS21, GW21, GYC20, JZL⁺21, PJ20a, PMdN21, RSD21, SDS19, SDS20, SBJ20, SG21, VdM22, WWM⁺21, ZLH⁺20b, ZZZ20b]. **Stabilization** [WWWC21]. **stable** [PAS⁺21, SZMM22, ZMS21]. **stacked** [Mok21c]. **stage** [KYL⁺20]. **stages** [DYK22]. **standard** [GSMT⁺20, WWL21]. **standing** [HZC21]. **Stark** [BAM20]. **State** [AKP22, MW21, ACM20, BXWK22, CZ21, CZW21, CPK22, DSNZ⁺20, Eti20, KGSD20, KYL⁺20, LFRTRP⁺20, LHL⁺21, Nag20b, NZ20, NZAH21, NYX⁺21, PGROM20, Rui22, SV21, SPR21, TSN⁺21, TVdVN21, ZHS21]. **state-natural** [LFRTRP⁺20]. **State-selective** [MW21]. **states** [CPL⁺21, DFB20, GDR21, Izs21, KK21, sLhZX⁺22, LBG20, Mka20, MM21, NHNO20, Nat22, RR21, Rui22, SBG21, SPR22, SKG21, TWT⁺21, TPB⁺20, TPCSD20, TT21b, TVdVN22, VGSS20, WY20, WWKH22, YÇDÖ21, dLRdLJ⁺20]. **static** [NHNO20, SFB20]. **Statistical** [LMMA21, Pev21]. **steel** [DPC⁺20].

Steiner [RMWF20]. **step** [LFMG20, WCZ⁺20]. **stepwise** [KZ21, WCZ⁺20].
Stereo [HYHW22]. **Stereo-dependent** [HYHW22]. **stereochemical**
 [MF21b]. **Stereodynamics** [WY20]. **stereoselectivity** [TXW⁺20]. **steric**
 [SC21, YCSK20]. **stoichiometric** [MSM⁺20]. **storage**
 [DRV20, KDY⁺22, KHH⁺21, LFX⁺21, RS21, RKA⁺21, RMeH⁺20, YZL21a].
Strain [LLZC20, tZNb⁺22, LXWZ21, WLY⁺20, YCPW20]. **Strain-tunable**
 [LLZC20]. **strained** [GMRKMC21, SC21]. **Strangely** [GOR20].
strength [BVL22, LAKJ20, ZZF22]. **strengths** [WWKH22, YÇDÓ21].
stress [MAMB⁺22]. **strong** [Dau21]. **Structural**
 [GYC20, JZX⁺20, JZL⁺21, KHH⁺21, LWH⁺21, MAHRA⁺21, MBM⁺21,
 NLA⁺21, PLT⁺20, RMM⁺22, AAM⁺20, AS22, AKK⁺21, BSS21, BB20,
 CMGH⁺21, DYG21, HNO⁺21, HBY20, KMG22, MSKA20, MKKA21,
 MKuAS⁺22, MK21, MIM21, MNWD20, MEWD20, ORL⁺20a, Pan20, PJ20a,
 Pan22, RPAA22, SUG20, SG20, TCSG⁺20, XFW⁺20, ZRR⁺21, tZNb⁺22].
Structure
 [BWLZ22, Kov20, YCSK20, AN20, AJC⁺21, BRB⁺21, BWBR21, CSY⁺21,
 CMM⁺22, DDSB22, Doh20, DLZ⁺21, EM21, FPdS21, FH21, GNC20,
 GXL⁺22, Gun21, HLL20a, JPSC20, KKH21, Kön21, LLW⁺21, MZD⁺20, PP21,
 RRD⁺22, RNA22, RNB22, RNFMC20, RKG21, SBA21, SBJ20, WXL⁺21,
 WWM⁺21, WP20, WFG⁺21, XBK⁺20, ZGCF20, ZHJ⁺20, ZMS21, tZNb⁺22].
Structure-activity [YCSK20]. **Structure-dependence** [BWLZ22].
structure-property [RNA22, RNB22]. **structure-reactivity** [CMM⁺22].
structure-toxicity [JPSC20]. **Structures**
 [JAZ⁺20, VCM⁺21, DCY21, ELH20, IAI20, KYL⁺20, LSG21, PZGH⁺20,
 ÜB20, WZ21, ZG21, ZZZ20b, ZZL20b]. **Strychnos** [SSK20]. **students**
 [BHH20, CM21]. **studied** [sLLqX⁺20, MZD⁺20, ORL⁺20b]. **studies**
 [AAN⁺21, BRB⁺21, CYJC20, GG20b, KLT21, SSEI21, SPR22, TCL⁺21,
 WWZ⁺20, WWM⁺21, WAW⁺21, XPZ20, XHX⁺20, ZL21]. **Study**
 [JXYL20, LZSA20, MM21, AAM⁺20, ASO⁺22, ABDD22, BBAA21, BMF20,
 BZP⁺20, BZW⁺21, BB20, Bra21, BSH⁺21, CCZ20, CZ21, CMGH⁺21,
 CPL⁺21, CMM⁺22, DRV20, DPC⁺20, DFK20, DLZ⁺21, FFBH21, FK20,
 FMH⁺22, dSFdSdMdM20, GB21, GNC20, GGUU21, HTNP21, HZC21,
 INV22b, JPSC20, JBPV21, JAZ⁺20, JZX⁺20, JSF⁺21, JWZZ20, KBR⁺20,
 KHH⁺21, KVCS21, KS21, LK20, LLLL20, LLW⁺21, LK21, LZ21, LG21,
 LWR21, LSS⁺21, MJA20, MZXL21, MSS22, MKKA21, MBKA21, MSKA21,
 MKKK22, MR21, MZF21, MAHRA⁺21, MI20, Mka20, MSADA21, MIM21,
 MM20, MHS21, MBM⁺21, MT21, NZ20, dAOdASP⁺20, PASS21, PSJ22,
 PGPHAPM20, PD22, RINH20, RSD21, RKG21, RC20, RED21, SPF⁺22,
 SFPH22, SBM22, SDL⁺22, Shi21, SG20, SRS21, STF21, SYT⁺21, TSN⁺21,
 TXW⁺20, THL⁺21, TSW⁺20, ÜB20, VSKG21, WLP⁺20, WZ20, WV20b,
 WXL⁺21, WLH⁺20, WHYL21, XZ20, XQJ⁺21]. **study**
 [XCZ⁺21, XWS⁺22, YZD⁺21, YZL⁺21b, YHW⁺22, YHZ⁺22, ZIA20,
 ZZZW20, ZZZ⁺20a, ZLT⁺20, ZLH20a, ZZLC20, ZXS21, ZKP22, ZZZ20b,
 ZZLY22, ZHS21, dLRdLJ⁺20, tZNb⁺22, YST⁺21]. **studying** [SC21]. **styryl**

[TPT20]. **styryl-bodipy** [TPT20]. **Subfemtosecond** [Mok21c]. **subjected** [Mok21a, NR21]. **subphthalocyanine** [CCZ20]. **subphthalocyanine-AzaBODIPY-C** [CCZ20]. **subsequent** [AAN⁺21, SYT⁺21]. **Substituent** [HLL20b, SSEI21, WLLS21, YCSK20]. **substituents** [BA21, DSNZ⁺20, LYT⁺20, PVR20]. **substitute** [YHW⁺22]. **substituted** [KM21b, ZXS20]. **substitution** [AAB22, CLL20, MEWD20, SSIE20, ZL21]. **subsystem** [GTV20, STN20]. **subsystem-based** [STN20]. **subsystems** [MJRS20]. **success** [Shi20]. **sufficient** [Sør21]. **sugar** [ZWW⁺22]. **suitable** [KJA⁺21, Pev21]. **sulfide** [FCL22, RDMF21]. **sulfonylimino** [NHNO20]. **sulfonylimino-** [NHNO20]. **sulfonyltriazoles** [WLH⁺20]. **Sulfur** [ZYZ⁺21b, MZF21, THS20]. **sulfur-doped** [THS20]. **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** [CSY⁺21, DLZ⁺21, VSKG21]. **Supramolecular** [SN21, CCZ20, RKG21]. **surface** [CXZ⁺21, LRG⁺20, LQZ⁺21, MC22, RHS⁺21, RK21, UBW⁺22, YZL⁺21b]. **surfaces** [DB20, HYY20, MBR21a, RKI20, SKG21]. **Sustainable** [KS22]. **SVECV** [VKK⁺21]. **SVECV-f12** [VKK⁺21]. **SVPD** [TCSG⁺20]. **swarm** [AJC⁺21]. **switch** [BMH21]. **switchable** [BS20]. **symmetry** [AIB21, BA22a, Rui22, ZZ22]. **symmetry-adapted** [AIB21]. **synergistic** [JHH⁺22, LXWZ21]. **synthesis** [CDG⁺21, LL20]. **synthesize** [Yan20]. **system** [AkAR⁺21, BGK⁺22, CZW21, KGSD20, MM20, PSJ22, SDS19, SDS20, YCL⁺22, ZFB⁺20, GG22]. **system-** [MM20]. **systematic** [GZC21, HMBPJ⁺20]. **systems** [AB21, CRC21, CFJ20, Cha21b, CSK21, CDR20, CSGR21, Gun21, Hua20, KZ21, Kön21, Lom21, PJ20b, RC20, SF20a, SPR22, SD20, VOK⁺20, Wan21, ZIA20]. **Szeged** [Ano22a, BT21, IMJ21a]. **Szeged-like** [Ano22a, BT21]. **Szeged-type** [IMJ21a].

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[GYC20]. **terbium-doped** [GYC20]. **terminal** [ZPS⁺20]. **Ternary** [LYW⁺20, KYL⁺20, WJF⁺21]. **terphenyl** [INV22b]. **terthiophene** [SV21]. **tested** [LAAP21]. **tetra** [LLMQ20, MM20]. **tetra-atomic** [MM20]. **tetra-N-heterocyclic** [LLMQ20]. **tetraazaacene** [FSR⁺22]. **tetraborate** [ZZL⁺20a]. **tetracoordinate** [TT21a]. **tetracyclic** [BDEM21]. **tetramerization** [YZD⁺21]. **tetraphenyldipyranilidene** [NIA21]. **tetrazine** [XWJ⁺21, ZJW⁺21]. **tetrazole** [ZZXT21]. **tetrazole-based** [ZZXT21]. **tetrazolo** [ZZXT21]. **tetrel** [HLL20b, LL21]. **tetroxide** [Kid21]. **Teukolsky** [CSS⁺21]. **their** [BRHECY⁺22, Boz21, ELH20, KKH21, LYFL21, LCX⁺21, LPH22, dAOdASP⁺20, ZLT⁺20]. **theorem** [Sør21]. **Theoretic** [IRA⁺20, OMA21]. **Theoretical** [AN20, ASHPHCB20, BBAA21, CYJC20, CBK⁺20, DYG21, FK20, GG20b, HBB⁺21, KWWZ20, Kan22, KKRR21, LWW20, LXZ⁺21a, LG21, LYTS20, LL20, LLMQ20, LLQ⁺21, LZZ⁺20, MSM⁺20, MFC20b, MI20, PSJ22, RG20, RDMF21, Roy20, SSIE21, SCZ21, SFPH22, SDL⁺22, STT20, SYL⁺21, SYT⁺21, TSW⁺20, WLP⁺20, WWZ⁺20, WZL⁺21, WSSD21, WAW⁺21, XPZ20, XHX⁺20, YYL21, ZL21, ZZLY22, AAM⁺20, BA21, CCZ20, Kid21, LZS20, LK20, LYT⁺20, MZXL21, MRI20, MWBQ20, MK21, Mka20, MOB21, dAOdASP⁺20, RINHY20, Röh21, SRS21, Yan21, YHZ⁺22, ZZ22]. **Theoretically** [ZWL22, RKI20]. **Theory** [BVL22, AIB21, ASO⁺22, ABDD22, ARRB⁺21, BBAA21, BZP⁺20, BRB⁺21, BB20, BWBR21, BSH⁺21, CLW21, CXZ⁺21, CPL⁺21, DRV20, DPC⁺20, DFK20, EGLJQ⁺21, FFBH21, GRFM20, GMO⁺20, GTV20, HLL20a, ID21, JZL⁺21, KZ21, KRS⁺21, KVCS21, KYL⁺20, Kön21, LLW⁺21, LK21, LCP21, LSS⁺21, MSKA20, MKKK22, MF21a, MSADA21, MAMB⁺22, MIM21, MP20, Nag20b, Nag22, NHNO20, PM22, PD22, Pev21, QdOdMC⁺21, QOM⁺20, RSD21, SSEI21, Sah21, SM22, SPF⁺22, SK20, STN20, SK21, SF20a, Shi21, SBJ20, SG20, STF21, Sur20, Sur22, TXW⁺20, THL⁺21, TCX⁺22, TAS21, WZ20, WAM⁺20, XZ20, XQJ⁺21, XWS⁺22, YZD⁺21, ZZZ⁺20a, ZXS21, ZS21, ZHS21, dPZFM⁺22]. **theory-based** [SK20]. **Theory/Polarizable** [BVL22]. **theory/time** [WZ20]. **theory/time-dependent** [WZ20]. **Thermal** [TCX⁺22, YHZ⁺22, ARRB⁺21, BRB⁺21, CMGH⁺21, CMM⁺22, FCL22, MKKA21, MWC⁺21, PKBZ20, WWZ⁺20, YFX⁺22, ZZLY22]. **thermo** [RKA⁺21]. **thermo-physical** [RKA⁺21]. **Thermochemical** [Iri20, Iri21]. **thermodynamic** [FAJOF20, GNC20, JZX⁺20, JZL⁺21, KMG22, LMA21, MBM⁺21, NR21, NLA⁺21, ONH⁺21, PL20, Pan22, PD22]. **thermodynamics** [YFX⁺22]. **thermoelectric** [AAB22, AAM⁺20, GSRG22, HBB⁺21, MTA⁺22, ONH⁺21, RMLPGHP20, TMH21, WWLL21, tZNB⁺22]. **thermomechanical** [UV20]. **thermophysical** [SG20]. **thiahelicenes** [KM21b]. **thieno** [PGPHAPM20]. **thiobarbituric** [LYT⁺20]. **thiolate** [PD22]. **thione** [dLRdLJ⁺20]. **thiophene** [MC22]. **thiophenol** [dLRdLJ⁺20]. **Three** [EPMC20, DKK⁺20, KMH⁺20]. **three-centered** [DKK⁺20]. **three-dimensional** [KMH⁺20]. **threefold** [Tia21]. **throughput** [XFW⁺20]. **thymine** [MHD20]. **Ti**

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wave [CPK22, Dau21, NZ20, PMdN21, STI20, Sør21, SY21, TVdVN21, TVdVN22]. **Wavefunction** [Höf21, CFJ20, NSM22, RKI20]. **wavefunction-in-DFT** [RKI20]. **Wavelength** [Hua20]. **Wavelength-decomposition-based** [Hua20]. **wavelengths** [WKH20]. **way** [BXWK22]. **weighted** [RNA22]. **well** [SD20]. **wells** [KRB20, Ole20]. **white** [ARBM21]. **Wiener** [ADZA21, Hao21, IMJ21b, Ye20, ZZL20b]. **Wigner** [TAS21]. **wiki** [Nag20a]. **wires** [YZY⁺22]. **withdrawing** [FFBH21, SCAD⁺20]. **within** [AMM21, HTNP21, HRA⁺22, LFRTRP⁺20, MKD21, QDOC⁺21, Rac21, RPT21b, STN20]. **without** [Cio22, ZHFD⁺20]. **WO** [JXYL20]. **women** [EPMC20]. **work** [WWM⁺21]. **Working** [PM22, TCL⁺21]. **worthwhile** [GTV20, SSEI21]. **WX** [SPF⁺22].

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

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Anonymous:2021:CIVk

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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:IIi

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Anonymous:2021:IIk

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Anonymous:2021:III

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Anonymous:2021:IIIm

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Anonymous:2021:IIIn

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Anonymous:2021:IIo

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Anonymous:2021:IIp

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Anonymous:2021:IIq

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Anonymous:2021:IIr

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Anonymous:2021:IIs

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Anonymous:2021:IIt

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Anonymous:2021:IIu

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Anonymous:2021:IIv

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Anonymous:2021:IIw

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Anonymous:2021:IIx

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Anonymous:2022:ESB

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Anonymous:2022:IIa

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- Anonymous:2022:IIc**
- [Ano22d] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(3):e26695:1–e26695:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).
- Anonymous:2022:IIId**
- [Ano22e] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(4):e26697:1–e26697:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).
- Anonymous:2022:IIe**
- [Ano22f] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(5):e26699:1–e26699:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).
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- Anonymous:2022:IIg**
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- Anonymous:2022:IIh**
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Biag:2022:SLE

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