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+ [BRW08, GAI08, TBM01]. 1.9$\AA$ [YKS+12]. 10 [AGO07]. 1s [LPC24, PTC+13, PTBH13, UYT97, VT24]. 2 [DAB+23, SRZE04]. 20 [AGO07]. 217 [Gos02a]. 21st [KvH99]. $2 \leq Z \leq 10$ [OE17]. 2×2 [KC19]. 3 [KMR01, SRZE04]. $3 + 1^1$ [SBK15]. 3d [MTA00, TSON00]. 5 [HBGvM19]. 5d [SED+98]. 5f^2 [MCC03]. 9 [JGCRC16]. = [HOI+08, KIT+08]. + [ARS99, BB14, KM98, SJO05, SM23, TM13]. − [CCM05, JMWG19, SEL01, TM13]. 1 [BRW08, VT24]. 13 [CPBS05]. $^1\Sigma_g^+$ [Kom05]. 2 [SP99]. 2+ [CLK15, Mam19, SCTH+07]. 2− [CSZ99]. 2h [DE05]. 3 [Bel19]. 3+ [ADA03, JSG+14, JS21]. 4+ [IOA03, TBM01]. 8 [RF13]. 9 [RF13]. • [PEMC23]. n [CPBS05]. $n+$ [LM03]. $n\pm$ [NM03]. $_0$ [MFMCN01]. $_1$ [SP99]. $_{1-x}$ [NIO03]. $_{1.75}$ [NM00]. $_{1/8}$ [GWM+03]. $_{10}$ [LC03]. $_{12}$ [HOI+08]. $_2$ [APNM03, BRW08, CSZ99, DLMS03, GP14, Hog18e, Hog21, Jan97, Lyo08, Mar08b, MCC03, Miy03, MKK+00, Mur03, NM00, OTA97, Sak03a, SP99, Sau05b, SH19, SCE19, SS04, SEL01, TMM03, YKS+12, YIYM03, ŻM23]. $_{2,3}$

[OTA97]. $_{20}$ [PM16]. $\frac{+}{2}$ [BMR+24, CLK15]. $\frac{-}{2}$ [Miy03]. $_{3}$ [CY00, CSZ99, DLMS03, GWM+03, HSS+04, IKN+08, JMWG19, KIT+08, MVL01, NeMM03, NIO03, NP03, OTA97, Sau05b, SSS05, YTC+05]. $_{33}$ [SMAS08]. $\frac{-}{3}$ [MGAUP23]. $_{4}$ [CL00, CSZ99, DA14, DLMS03, Jan97, OM03, RZTSW23, Sau05b, SIY+19, YKS+12]. $_{5}$ [SIY+19, YKS+12]. $_{5 \leq n \leq 8}$ [RK04]. $_{6}$ [APNM03, ADA03, CSZ99, HOI+08, KDG97, MKK+01]. $_{60}$ [LM03, NM03, PEMC23, SCN03]. $_{67}$ [SMAS08]. $_{7}$ [CL00]. $_{7/8}$ [GWM+03]. $_{c}$ [DB01]. $_{n}$ [CMVPFC16, UMD08]. $_{x}$ [NIO03]. $_{X \text{ — } Y}$ [DE05]. α [Ada97b, Ada00, CL00, FSB+97, Fuk03, GG20, Gut97, IFAY08, Kaw97, KNM+08, LSZ+00, MYW00, MW08, MKK+00, MTA00, Mur08, Nak00, NHYU03, OTA97, Ros97, SBA+03, SBK+08, SNMI00, SYIY03, Tan00, UMD08, YFK+97]. B [ZBM98, Wen21]. β [CCT02, DNM+14, KS88, MTA00, RMN+14, dLHD10]. β^- [RF13]. : [ADA03]. D [Apo01, BG23, DB01, CCA13]. d^5 [DST+03]. $e^{\pm}$ [HHU+21, WHB+24]. E_i [HHU+21]. f [BKC68]. g [MWL+05, SJO05, Sau05b]. $G \otimes (g \oplus h)$ [LPDB03]. $H \otimes 2h$ [LC03]. I [ZBM98]. $J > 0$ [ACDV01]. K [GVFR98]. L [HMH+18]. $\leq$ [HHU+21]. $\leq E_i \leq$ [WHB+24]. M [HMH+18]. $\mu - S_2$ [CSZ99]. N [LK90, CMVPFC16, Gal73, GSTvE98, RRMAF08, VT24]. ns [VT24]. p [BK70, CCCC15]. π [FH65, Fow03, Ohn67]. $\psi^{(\alpha*)}$ [AFE13]. q [KMR01]. R_3 [MKB04]. s [GW01]. s^2 [AR03]. Σ^+ [SZP21]. T [AHPD+03]. T_3 [MKB04]. $T \otimes (e \oplus t_2)$ [LPDB03]. Y [BMC97]. Z [SGK+08, DTC04].

-2-azabuten-4-yl [NeMM03]. **-Al** [OTA97]. **-Bromopropane** [RRMAF08]. **-Bromouracil** [HBGvM19]. **-Carboxylic** [JGCRC16]. **-carotene** [CCT02]. **-Cyclodextrin** [DNM+14, RMN+14, dLHD10]. **-Decay** [RF13]. **-Decay-Induced** [KS88]. **-Deformed** [KMR01]. **-Dimensional** [CCA13, KMR01]. **-doped** [IOA03]. **-Edge** [OTA97]. **-Electron** [FH65, Gal73]. **-ETOs** [AFE13]. **-Family** [DLMS03]. **-helices** [GG20]. **-K** [KC19]. **-lone** [AR03]. **-Method** [FSB+97]. **-Nitroaniline** [CCCC15]. **-Parameter** [Apo01]. **-Particle** [GSTvE98]. **-Phenyloxirane** [JJD05]. **-Representability** [LK90]. **-Schrödinger** [BG23]. **-site** [DAB+23]. **-States** [BK70]. **-Subshells** [HMH+18]. **-Tartaric** [HSR98]. **-Type** [GW01]. **-Values** [BKC68]. **-Wave** [DB01].

/Ã [SP99]. **/alumina** [Hog23c]. **/K** [MTA00].

0.1-2 [Sim07].

1 [BG23, HHU+21]. **1-** [NeMM03]. **11-tetraazacyclotetradecane** [MYW00]. **1s** [HPB17].

2-azolyl [NeMM03]. **2-bis** [YKY+00]. **2-Cyclohexenone** [GBHM14]. **2-Hydroxy-acetamide** [SDGW98]. **2012** [Hog13g, Hog14].

3-Dipolar [RGA99]. **3P** [RT18].

4-Center [AA18]. **4-dioctyloxyphenyl** [YKY+00]. **40** [Miy03].

= [BMC97, BJMB14, CMVPFC16].

A1N [SYIY03]. **Ab-Initio** [DO09]. **Absolute** [MYM08]. **absorbed** [LYM03]. **Absorbing** [RDNFH98]. **Absorption** [CCCC15, CLÅ05, JGCRC16, Jos08, KsKsN08, KNM+08, MYW00, MW08, Mur08, Tak19, YFK+97, IOA03, Mur03, SP99, YNNU03]. **Abstract** [KS97b]. **academic** [SBK+08]. **Accelerating** [ST07, BG23]. **Accounting** [DKV+19]. **Accumulative** [BR65]. **Accuracy** [BR65, Hal64, KE98, Koł70, Pau13, Ros97]. **Accurate** [BC80, CS77, SZP21, ŚBG14, Bis19, EÜSB21, KHPP23, LH20, VT24]. **Accurately** [Hog18e]. **ACES** [PM16]. **acetamide** [SDGW98]. **Acetic** [PWZ+08]. **achiral** [QSW20]. **Acid** [BWH08, HSR98, JGCRC16, KLG+08, KV08, PWZ+08, Tur07]. **Acid-Water-Ammonia** [KV08]. **Acidities** [Sey12]. **Acids** [PP68]. **Acknowledgement** [Ano04a]. **Across** [DE05]. **Acrylonitrile** [RGA99]. **Actinyl** [HTS+00]. **Activation** [Bro98a, Bro98b, OM03, RZTSW23]. **Active** [Bro98a, Bro98b, YMI+21]. **Activity** [Jan97, ST17]. **Adaptation** [KCM70]. **Adapted** [KMJ97, CAG+21, KHPP23]. **ADC** [Hät05]. **Adding** [Sim05]. **addition** [KBH23, PEMC23]. **Adiabatic** [AdMB99, BVHK03, DST+03, JSG+14, Koł70, ML18, Nag01, NFW+98, SJO05, Sim99, BMR+24, JS21]. **Adjoint** [Löw96b]. **Adjustment** [LJK+08]. **adsorbed** [Hog21, HDFT24, KBH23]. **Adsorption** [GBHM14, SN08]. **Adv** [Miy03]. **Advanced** [BKB+19, MK23, YKC+08, SBA+03]. **Advances** [ABC+98, Ano13a, Ano13b, Ano19a, BSB13, Brä21a, BB22b, BB24a, Cam12, CS04, HPL98, Hog13a, Hog13b, Hog18b, Hog23a, JKMB19a, Löw64a, Löw65a, Löw67a, Löw68a, Löw70a, Löw72a, Löw73a, Löw74a, Löw75a, Löw77a, Löw78a, Löw80a, Löw81a, Löw81b, Löw82a, Löw82b, Löw85a, Löw86a, LSZ88, LSZ89, LSZT90, LSZ91, LSZ92a, LSZ92b, LSZ94, LSZ95, LSZ96, LSZ+97b, LSZ+97a, LSZ+98b, LSZ+98c, LSZ+98a, LSZB99, LSZ+99b, LSZ+99a, LSZ+00, LSZB00, MPU19, NBS10, SBM+01a, SBM+01b, SB02, SBA+03, SB03, SBC+03, SBCT04a, SBCT04b, SBK04, SO05b, SB05, SBLJ05, SB06, SB07, SBSL08, SBK+08, SBGJ08, SBC09b, SB09a, SBC09a, SBC10, Sab11, SB11, SB12a, SB13a, Sab15, SB17a, SB17b, SB18a, SS99, AP03, SSK03]. **Advancing** [LÖS02]. **Advantages** [HB14]. **Adventurer** [OS05, SO05b]. **Advisory** [Ano94a, Ano98a]. **Aerosol** [KSG08]. **Affect** [Tak19]. **Affinity** [KDG97, Bel19, GPEB21]. **after** [MBAPS19]. **Ag** [ARS17, SHBC19, WHB+24]. **Aging** [Löw65c]. **Aharonov** [Sjö04]. **Al** [KBH23, KKA97, MGAUP23, OTA97, WHB+24]. **alcohol** [GC01]. **Algebra** [LMSP01, Löw92a, Pal04]. **Algebraic** [AČP88, FMA08, QGW01, WN05, Yas17, Yas23]. **Algorithm**

[ACDV01, Kou15]. **Alkali** [Jan65, ML18, SCN03, Tak19, SJAB+22, STO+00]. **Alkali-Metal-Doped** [SCN03]. **Alkaline** [KRL01, STO+00]. **Alkaline-Earth** [KRL01]. **Alkyl** [PL98]. **All-Electron** [MSM17]. **all-metal** [MGAUP23]. **all-particle** [SA23b]. **Alleged** [Sjö04]. **Allosteric** [ST17]. **alloyed** [TMM03]. **Alloys** [KKA97, MLR+98, YM00]. **Almost** [LGJP99]. **Almost-Linear** [LGJP99]. **Along** [BŚG17, Nag01]. **Alpha** [BRL13]. **Alphas** [Sab97]. **Alternative** [Ave98]. **alumina** [Hog23c]. **Aluminate** [MW08]. **aluminium** [PGV97]. **aluminum** [CCL03, Hog21, MST+03]. **Ambient** [ASGG08]. **amine** [NeMM03]. **Ammonia** [KV08]. **among** [IFAY08]. **Amorphous** [Mur08, SMAS08]. **analogy** [YMI+21]. **Analysis** [Ada00, Bel11, BE04, BRL13, Fuk08a, HSR98, KÖO23, Kle77, Len68, Löw92a, Mur08, Nal00, Nic10, OTA97, SJO05, STO+00, Shi12, Sid18, SYIY03, TP03, Uda00, UMD08, WmG18, YKC+08, Bis19, CCM+19, IOA03, MST+03, Sak03a]. **Analytic** [BGW73, BG73, Gre73, OE17, ZP17]. **Analytical** [Brä12, Cam12, CH03, GC10, GC92, HPU+17, HJ88, Lin17b, Rui23, WN05, BB21]. **Analyzing** [Köv08]. **Angles** [CLK15]. **Angular** [Har05, MFLK15, WP06]. **Anharmonic** [EÜSB21]. **Anion** [Lin05, Bel19, MGAUP23]. **Anionic** [RK04, JMWG19]. **Anions** [Fuk15, Sim99]. **Anisidine** [DNM+14]. **anisotropy** [ZLL+20]. **annihilating** [AP03]. **Annihilation** [FJS+04, SSK03]. **Anniversary** [Ano03a, Ano19b]. **Announcement** [Ano88a, Ano89a, Löw88a]. **ANO** [AT91]. **Anomalies** [GMP98]. **Anomalous** [HBKS03]. **Ansatz** [TA04]. **Answer** [Miy03, SEL01]. **Anthracene** [JGCRC16]. **Anthracene-** [JGCRC16]. **Anthropogenic** [AVB08]. **Antibinding** [FRM70]. **Antiferromagnetic** [Fuk08a]. **Antiferromagnetism** [Fuk15]. **Antihydrogen** [FJS+04]. **Antilinear** [SS03]. **Antimatter** [Gre08, Fro02]. **Antimatter-The** [Gre08]. **Antiproton** [PBK04]. **Antisymmetric** [Sal74]. **Antisymmetrized** [Wei04]. **AO** [CB92]. **Aperiodic** [Löw65c]. **Apology** [The96]. **Appendix** [Gos02a]. **Applicability** [DSW04, SIY+19]. **Application** [ASGG08, AGL05, AR03, CH03, Dru78, GC92, GW17, HPB17, KE97, Lin17c, Öhr17, PM16, PL98, RPSB00, Ray95, Rei73, Tan00, WD70, YMI+21, YTC+05, MKK+01]. **Applications** [AČP88, ABB90, CCSZ01, EG99, HM21, JG08, LB92, MNR+98, OE17, PSAP10, SBGJ08, SSV98, SGM+13, Sva98, ZLC+10, BPK23, Hog14, NBS12, PBOL02, Ros97, LFM89]. **Applied** [Byl98, Cru09c, OO05]. **Applying** [SSCL97]. **Approach** [ADRAB16, AL04, BKB+19, Chi03, CH03, CHSC03, CC97, DGKCT15, DR90, FMA08, GMLSC+10, GC10, Glu19, GCAGM17, HPRR10, HL90, IM80, KMHL13, Kob68, KD11, Ler85, LHL18, Löw85c, MH98, McW98, MKN10, MM99, NAY+08, NFW+98, Oli12, PČ75, PTC+13, Pul77, SG80, TA04, Tap09, dLHD10, vL03, EW03, MU03, SA23b, SKS+19, Zap01]. **Approached** [vS07]. **Approaches** [BBB10, KB86, LvWH+01, MC10, PGP17, STZY18, SS99, CTC22, JS21, Ort22, WLM23]. **Approaching** [CCC17]. **Approximate** [KB98, LGJP99, Lin02, MKB04, Nes67, PJH05, RAR15, MPU19, QSW20].

Approximating [HPB17]. **Approximation** [BG73, CHR13, Hur73, Koł70, Lyk64, NA04, Pol03, QGW01, SED+98, Sid18, BG23, GWW19, Köv03]. **Approximations** [BB99b, LV90]. **Aqueous** [BWH08, CCM05, MYW00, MW08, PWZ+08, dLHD10, MST+03]. **Arbitrary** [LR72]. **Architecture** [PWZ+08]. **Architectures** [Oli12]. **Aromatic** [AVB08, DSW04, FLV99]. **Aromaticity** [Ran18, MGAUP23]. **aromatics** [RZTSW23]. **Arsenide** [KSY08]. **Art** [AdMB99, AH19b]. **Artificial** [Duc97, MP22, SSCL97, YMI+21]. **Aspects** [ACDK72, Bis94, Coh04, Dau70, DDPC95, Fow03, GEO91, KK85, Löw65c, Löw85c, Löw98, PP68]. **Assessment** [BB99b]. **Assignment** [CÅ01, NM00]. **Assisted** [ALND10, DBC+99, PLA01, Dra20, MS03]. **Associated** [Löw88b, LFM89, OTA03]. **Asymmetric** [MFLK11, ORL23]. **Asymptotes** [HM21]. **Asymptotic** [BE04, JSF08, KKGG98, LRCR98, SPH14, Sid18, BKL21]. **ATiO** [KIT+08]. **Atmosphere** [ASGG08]. **Atmospheres** [JGNJ08]. **Atmospheric** [BRW08, GAI08, JG08, KSG08, KLG+08, KV08, MCG+08, Mar08b, NAY+08, ZZ08, SBGJ08]. **Atmospherically** [ILS08]. **Atom** [Bel09, BMM13, CTO18, Cru09c, FVB99, FAS+98, GV09, GW18, HG17, Jan65, KO18, Kle77, KMJ97, Lau09, LK09, MFLK11, Mic15, Mic17, RT18, RAR+08, STZY18, Bar23, Bel22, JS21, Mic02, Mic22, MBAPS19, NA19]. **Atom-by-Atom** [FVB99]. **Atomic** [AFE13, AJ04, AT91, ADRAB16, AAAC04, BS98, BKC68, Bli65, CCA13, DKMP98, DY08, Dru78, DKV+19, Eks98, GP91, Glu19, GM91, Hal64, HPU+17, HMH+18, Har18, HOI+08, HM21, Hyl64, KS77, Kob68, KGI+19, LK13, Lin17c, LA12, MG22, Nor98, OPPZ06, Ono00, PR98, RLF17, San98, SOS15, SBF+08, SCM09, Ste73, TSON00, TAM04, WMM+98, Bun23, CTC22, CAP19, HPL98, LSZ+00, NBA20, RSP21, SBSL08, SKK23, SA23b]. **Atomic-Beam** [Eks98]. **Atomic-Number** [Ono00]. **atomicity** [BFHS23]. **Atomization** [PEZB98, SYM+08]. **Atoms** [AAE+01, AAM04, Ano08h, Aqu09, ACDK72, AA05, BND81, Bad09, BGW73, BG73, Byl98, Dol09, DGKCT15, ERC88, FSB+97, FMA08, Glu19, GSTvE98, Gre73, GVFG09, HUS+11, IS01, JSF08, Jan65, Jør74, KRL01, KMJ97, LASV18, ML18, Mat96, MKN10, Nes75, Nic10, OE17, PV09, PJH05, Phi98, RR05, RP18, RRMAF08, RF13, Saa01, YTF78, BH24, CM24, FCAG19, FTG22, GW23, HHU+21, MKK+01, SJAB+22, Tők19, WHB+24]. **Attachment** [JA07, SSS05]. **Attempt** [FHHE82, Zap01]. **attochemistry** [SBH+20]. **attosecond** [WLM23]. **Auger** [ÅCL92, Köv03, Köv08, MM96]. **Augmented** [SED+98, Sla64]. **Author** [Ano64a, Ano65a, Ano67a, Ano68a, Ano70a, Ano72a, Ano73a]. **Autoionizing** [AA05]. **Automated** [WN05]. **automatic** [Bun23]. **Auxiliary** [Per98a]. **Average** [GMLSC+10]. **Averaged** [ILS08]. **axons** [JJ20]. **azabuten** [NeMM03]. **Azide** [PL98]. **Azido** [IFAY08]. **Azido-Bridged** [IFAY08]. **azolyl** [NeMM03].

B [HOI+08, Miy03, SP99, Mam19, SCT16]. **Ba** [KIT+08, GVFG09]. **Back** [Lin17b]. **bacteriophytochromes** [Dur20]. **Bad** [QSG98]. **BAg** [BU97]. **Balance** [PM14, Vis05]. **Band** [Cse97, KSY08, Kri03, PGN04, SS90, Sla64, SSV98]. **Band-Structure** [PGN04]. **Bands** [BWK97]. **Barkas** [Por04]. **Barkas-Effect** [Por04]. **Barnett** [SPH14]. **Barrier** [Hog18e, PEZB98, PLA01]. **Base** [JA07, KN01]. **Based** [ATL+18, AR03, BB13, GEO91, HZ89, KS97b, LFM89, OTA97, OYI+00, WmG18, BSL+19, SRZE04, YNNU03, ŻMM23]. **Bases** [CL07, MFLK15, PP68]. **Basic** [AYÖ17]. **Basicities** [Sey12]. **Basis** [AT91, AH19b, BL18, CTSOS99, Dau64, Gil94, GW01, IM80, MW98, Mon05, OOSS17, PTC+13, Pul77, QGW01, SPAS05, SW98, SDGW98, VWP+98, WM97, CCM+19, CAG+21, CAP19, GW23, RA19, SKGŚ23, Wen21]. **BaTiO** [CY00, IKN+08]. **Batteries** [YKC+08]. **BAu** [BU97]. **BC** [ACDV01, Mur03]. **BCu** [BU97]. **Be** [RLF17]. **Be-Like** [RLF17]. **Beam** [Eks98]. **Beginnings** [HKS90]. **Behavior** [ARS17, JSF08, KG12, Lev14]. **Behaviour** [LRCR98]. **Benchmark** [MWL+05]. **Benford** [MG22]. **Benzene** [JH99, KBS03, LGK+99, RAR+08]. **Bersuker** [Ano03a]. **Bessel** [HPB17]. **Bethe** [CTSOS99, ORL23, Por04]. **Between** [FLV99, GV09, KMJ97, OBHM17, Suc98, AR03, BVHK03, LR72, Nal06, PMK23, RR05, Ste73, VG22, YMI+21]. **Beyond** [GS04b, Lin98, HO16]. **Bi** [LFM89, KNI+08]. **Bi-Variational** [LFM89]. **Bimolecular** [Sko12]. **Binary** [MKK+00, MYM08, LCC22, TSTH03]. **Binding** [FRM70, KRL01, PEMC23, Ort22, PGV97]. **Biogenic** [ZZ08]. **Biographic** [Ano99a]. **Biological** [AGMdV+13, BGG+07, Bic13, Löw65c, MBO+07]. **Biology** [FHHE82, Rei73, SL20]. **Biomolecules** [HS19, JJD05, Sab07, SOS11, Bel21, SB07]. **Biophysics** [Jeh65]. **biosynthesis** [Hes22]. **Biphospholylidene** [PM16]. **Bipolar** [Sil14]. **Bipolaronic** [DB01]. **Birefringences** [RC05]. **Bis** [YKY+00]. **bisphenol** [BTB+20]. **Bivariate** [Lev14]. **Black** [Mur08]. **Bloch** [Löw98, Por04]. **Blocks** [Brä04]. **Board** [Ano88d, Ano89d, Ano90c, Ano91c, Ano92e, Ano92f, Ano95c, Ano96d, Ano97f, Ano97g, Ano98m, Ano98n, Ano98o, Ano99i, Ano99j, Ano01i, Ano03g, Ano08g, Ano09g, Ano09h, Ano10e, Ano10f, Ano11e, Ano12e, Ano19i, Hog13e, Ano99k, Ano13e]. **Body** [AAE+01, AA01, BMM13, BŚG14, DDPC95, FP06, GAM+13, Har04, Har05, HA13, Har17, HW01, HMW01, Khe19, KT98, KB86, KO19, MC10, Mat78, MK18, SW98, Shi12, WDD16, vL03, BKL21]. **Bohm** [Sjö04]. **Bohmian** [GMB04]. **Bond** [Apo01, CCSZ01, CS04, DE05, GVCN82, Joh73, Krs16, Nak00, NSM11, San92, SH95, SKT+08, SYM+08, SSS05, TLOK97, YM97, BLC23, OTA03, STO+00]. **Bonded** [FCC04, GAI08]. **Bonding** [Bra67, HTS+00, KTMA08, LK14, Lin05, MC10, Ono00, Ort99, PWZ+08, SH95, SIY+15, SMAS08, TSON00, WD70, BFHS23, LYM03, NHM03, ŻMM23]. **Bonds** [DE05, Nal09, She15]. **Boranes** [BMC97]. **Born** [TA04, BG73, CHR13, NBA20, SZP21, SA23b, Tap01]. **Boron**

[BU97, HOI+08, Oli12, Bel19]. **Boron-Coinage** [BU97]. **Both** [RC05, CTO22]. **Bottom** [Oli12]. **Bottom-Top** [Oli12]. **Bound** [AAE+01, CTSSO19, KO19, RLF17, Shi12, CBSM20, JMWG19, RA19]. **Boundaries** [Cru09c, LK09, PB20c, OTA03]. **boundary** [Bel22, Sak03b]. **Bounds** [GP91, Wei72]. **Boxes** [Aqu09]. **Br** [FPL97, HOI+08]. **brain** [NTT20, PB20a]. **Breaking** [Apo01, She15]. **Breakings** [Ber03]. **Breaks** [Sim07]. **Breit** [LT98]. **Bridged** [IFAY08]. **Brillouin** [HW01, HMW01, MH98]. **Bromine** [FPL97]. **Bromopropane** [RRMAF08]. **Bromouracil** [HBGvM19]. **BSSE** [VWP+98]. **Built** [RP72]. **bulk** [SKK23].

C [CPBS05, CSZ99, BMC97, CTSSO19, JMWG19, LM03, NM03, PM16, PEMC23, SCN03]. **Ca** [CY00, GVFG09]. **Ca-Doped** [CY00]. **Cage** [Kat03]. **Cages** [CKC09]. **Calculate** [GM05]. **Calculated** [AA05, Hal64, PJH05, VWP+98, NHYU03]. **Calculating** [Dau64, SA23b]. **Calculation** [Ada97a, Ada97b, CTSOS99, CTSDÖ04b, CL00, DKMP98, FCH15, Gal73, GDL98, GSTvE98, HJ88, IOI+00, IFAY08, Kaw97, Khe19, KNI+08, KSY08, McG04, MKK+00, OE17, PR05, PBK04, SPAS05, SP99, SSO19, TMN10, YKC+08, YTC+05, IOA03, KTA03, MAS03, SH19]. **Calculations** [ÅVM96, AFE13, AT91, ABGM03, ASGG08, AAG03, AAAC04, BGW73, LJK+08, BC80, Bis94, BR65, BŚG14, CMFA99, Chr72, DRV82, DDPC95, DA14, EEL96, EM17, Fuk00, Fuk15, GVCN82, HSS+04, HBT+00, Hog18e, IKN+08, IS01, JMWG19, KE98, KNM+08, LF09, Löw80b, LÅJM95, MYW00, MWL+05, MK18, MCM14, MSM17, Nes67, Odd78, OTA97, OYI+00, Ohn67, ÖB81, PS05a, PTC+13, PB75, PL98, PWZ+08, QGW01, San92, SJO05, SED+98, SNMI00, SIY+15, Sla64, ŚBG14, Tan00, Uda00, UMD08, VI01, YFK+97, ZDZO11, vS07, AP03, Bun23, Fuk03, GW23, MOB+03, NBA20, PS21, PMK23, RA19, Ros97, SM23, SSK03, Yam03, YNNU03]. **calculus** [Ber02, VT24]. **CaMn** [SIY+19, YKS+12]. **Can** [MRS+99]. **Cancer** [BB11]. **Canonical** [CDK15, LB92, MDÖ05]. **CaO** [TP03]. **Capacity** [MYM08]. **caps** [LC03]. **Capture** [LK13, MA04, MTA00, Bel21, MG22]. **Car** [PWZ+08]. **carbide** [RZTSW23]. **Carbides** [SNM+97]. **Carbon** [BRL13, Mur08, RT18, LYM03, MOB+03]. **carbonitriles** [JMWG19]. **Carboxylic** [JGCRC16]. **Career** [Nor98]. **Carlo** [AGL05, CCT02, CCM05, CC97, HB14, Hog18e, Hog21, Hog23c, HDFT24, KBH23, MCA+18, NFW+98, RMMP17, RP18, SH19, TAU17, vS07]. **Carlo/Quantum** [CCM05, CCT02]. **carotene** [CCT02]. **Cartesian** [CB92]. **Cascade** [HS19]. **Case** [GVFR98, HOI+08]. **Cases** [CHSC03]. **CASSCF** [CTG98]. **CASVB** [CTG98]. **Catalysis** [Bro98a, Bro98b, Hog23c, KBH23]. **catalyst** [Hog21]. **Catalysts** [HB14, Hog18e, LDP+04]. **Cation** [KBS03, LGK+99, OTA97, LMK19, TMK21]. **Cationic** [DNM+14, RK04]. **Cations** [ARS99, CL07, KTMA08, CTSSO19, FB20]. **Cauchy** [PJH05]. **Cause** [Sim07]. **Cavity** [CTO18, Lau09]. **CC2** [Hät05]. **CC3** [PJH05]. **CCSD** [BB99b]. **Cd** [HHU+21]. **CdI** [BKC68]. **Ce** [NM00]. **Cell** [BB13].

Cells [KD11, GTB23]. **Cellular** [BB15]. **Center** [AA18, Bis67, CB92, ZP17, Rui23]. **Century** [BB99a, KvH99]. **CeO** [NM00]. **Ceramic** [Fuk00]. **Ceramics** [CY00, Tan00, Sak03b]. **CETO'S** [CB92]. **CF** [UMD08]. **CH** [MVL01, RZTSW23, Sau05b]. **Challenge** [RC05]. **Challenges** [DC99]. **Change** [FU00, Löw88b, LFM89]. **Changes** [YKY+00]. **Changing** [HB14, LA12]. **Channel** [Les75]. **Channeled** [GP04]. **Channels** [Sch94, SIY+15]. **Chaotic** [IBB+19]. **Chapter** [BMR+24, BH24, CM24, HDFT24, Kar24, LPC24, VT24, WHB+24]. **Character** [NeMM03]. **Characteristics** [SKT+08, YM00, SSK03]. **Characterization** [DDPC95, MM96]. **Charge** [BLKS78, CHR13, CCSZ01, CS77, FLV99, HPRR10, Jeh65, JS21, KKA97, LA12, MF04, OYI+00, SCTH+07, Bel22, GJP23, TBM01]. **Charge-Changing** [LA12]. **Charge-Transfer** [FLV99]. **Charged** [Ano08h, Ano08j, AK12, CHR13, KH03, LT98, PGN04, Sig05, TTLB04, AGS+19, BKL21, Tők19]. **Charged-Particle** [Sig05]. **Charges** [NA04, OPPZ06, SKK23, WD22]. **Charles** [Sab00]. **Chem** [Miy03]. **Chemical** [AT91, ACC99, BS04, BR20, Cal13, CT82, Dau67, DW98, FF72, GDL98, Gut06, HTS+00, Joh73, Jør74, JGNJ08, Kar97, KTMA08, Kuk14, Ler85, MÅ01, MM99, Nal03, NSM11, NHM03, Ono00, Ort99, PSAP10, RNL14, SJO05, Sey12, SH95, She15, SKT+08, SYM+08, SW81, Sko12, Sla81, SGM+13, TMN10, TSON00, Tap01, Tap09, WD70, YM97, BPK23, Brä03, BFHS23, LYM03, PBOL02, STO+00, ŻMM23]. **Chemical-QSPR** [Sey12]. **Chemisorption** [SG80]. **Chemistry** [AVB08, Ano04l, Ano13a, Ano13b, Ano19a, Bel11, BSB13, BR20, Brä21a, BB22b, BB24a, CCC17, CS77, CB18, Cra99, DKV+19, Duc97, EBR92, FHHZ88, HPL98, Hog13a, Hog13b, Hog18b, Hog23a, Jan65, JKMB19a, KS97b, Kla81, KV08, LBH+17, Lar17, LDP+04, Löw64a, Löw65a, Löw67a, Löw68a, Löw70a, Löw72a, Löw73a, Löw74a, Löw75a, Löw77a, Löw78a, Löw80a, Löw81a, Löw81b, Löw82a, Löw82b, Löw85a, Löw86a, LSZ88, LSZ89, LSZT90, LSZ91, LSZ92a, LSZ92b, Löw92a, LSZ94, LSZ95, LSZ96, LSZ+97b, LSZ+97a, LSZ+98b, LSZ+98c, LSZ+98a, LSZB99, LSZ+99b, LSZ+99a, LSZ+00, LSZB00, MCG+08, MRS+99, Mat64, Mez96, MP97, MG23a, NAY+08, NBS10, Nic11, OS05, Oli12, Oni12, Oni15, OO82, Pyy78, QSG98, Ryc98, SBM+01a, SBM+01b, SB02, SBA+03, SB03, SBC+03, SBCT04a, SBCT04b, SBK04, SO05b]. **Chemistry** [SB05, SBLJ05, SB06, SB07, SBSL08, SBK+08, SBGJ08, SBC09b, SB09a, SBC09a, SBC10, Sab11, SB11, SB12a, SB13a, Sab15, SB17a, SB18a, SSCL97, SBK15, Sut98, Tap17, VWOS89, BB21, Dra20, Fro02, Hog14, HO16, LÖS02, NBA20, SCT15, SCT16, SB17b]. **Chiral** [LDP+04, QSW20]. **Chirality** [CL05]. **Chirped** [CM24, MCP12, ML18]. **chromium** [CCL03]. **Chromophore** [BHM17]. **CI** [Ave98, BE01, Har18, PB75, RSP21, Rui23, TR98]. **Circular** [CE72, PR05]. **Circulenes** [SKT+03]. **Cl** [RAR+08, CTSSO19, RRMAF08]. **Cl-Atom** [RAR+08]. **Classical** [AdMB99, GMB04, HM19, MT04, Per20, PS05b, PSAP10, Sig05, Sim99, WDD16, BPK23, EW03]. **Classical-quantum**

[Per20]. **Classification** [FHHE82]. **clean** [SH19]. **close** [JS21]. **close-coupling** [JS21]. **Closed** [Bra77, Cru09c, JSF08, KRL01]. **Closed-** [Bra77]. **Closed-Shell** [JSF08]. **Closed-Subshell** [KRL01]. **Cluster** [Ada97a, Bra77, Cam12, CL00, FP06, GEO91, HJ99, HS86, KE97, KE00, KB86, KMR01, LEK01, LGJP99, MDBM98, MH98, MP89, MMSK16, MSM17, OTA97, OYI+00, PJH05, PM16, PB99, RR05, ST17, SB99, SIY+19, SG80, WN05, YKS+12, BPK23, CCM+19, EÜSB21, Fuk03, GWW19, GPEB21, Köv03, LMK19, MKB04, MK23, TMK21, TM21]. **Clusters** [BHV+00, Bor03, CMVPFC16, EGCL91, HL97, HOI+08, ILS08, Kap98, KRL01, KIHA97, LJ17, MLR+98, RK04, RMMP17, Saa01, Tak19, EOH03, Fuk03, LSZ+97a, STO+00]. **CO** [HB14, Hog21, HDFT24, KBH23, SNMI00, CMVPFC16, FU00, NHYU03, Yam03]. **Co-** [NHYU03]. **Coalescence** [KNN17]. **Code** [SGM+13]. **Codes** [Pau13]. **Coefficient** [MYM08]. **Coefficients** [ASGG08, HJ99]. **Cognition** [SS17]. **Cognitive** [Sri01]. **Coherence** [TS10, CM24]. **Coherent** [GP04, Ram98, RAR15, Wei04, WMM+98]. **Coinage** [BU97]. **cold** [ŻM23]. **Collective** [BS72, SCE19, JJ20]. **Colliding** [Saa01]. **Collinear** [Per98b]. **Collision** [Les75, MMM19, Tők19]. **Collisional** [BKB+19, MHWvdA97]. **Collisions** [AGMdV+13, Bel09, BMM13, BR17, BB14, CHR13, CCSZ01, DGKCT15, FAS+98, FJS+04, KMHL13, Kle77, LK13, Mic74, MF04, MM13, RGFC13, SCTH+07, Bel21, Bel22, JS21, TBM01, ŻM23]. **Colour** [VTM98]. **Combinations** [LDNP99]. **Combined** [KBS03, LGJP99, TMN10, TL10, MKK+01]. **Combining** [MP97, SBC10]. **Combs** [MCP12, ML18]. **Comment** [Miy03]. **Communication** [Nal09, NSM11]. **communications** [Nal23]. **Compact** [HS05, VT24]. **Companions** [Cra99]. **Comparative** [BRL13, GV09, JJD05, KIT+08]. **Comparison** [BKC68, LvWH+01, Löw98, PS05a, QGW01, RR05, Sau05b]. **Competing** [Dur20]. **Competition** [PMK23]. **competitive** [SCJ+23]. **Complete** [CCA13]. **Complex** [Byl98, DST+03, LBH+17, Löw88b, LFM89, NeMM03, Nes75, STZY18, SIY+15, SIY+19, Ste73, YAJHR03, YTF78, ALA21, ALA23]. **Complexation** [ARS99]. **Complexes** [DB68, JA07, Mam19, MYW00, MHWvdA97, YFK+97]. **Component** [SW98, YZDM01, Bar23]. **Components** [AGO07, QSG98, BB22a]. **Composed** [PTC+13]. **Composition** [MKK+00]. **Compounds** [AVB08, Ber74, GAI08, HSR98, IFAY08, LvWH+01, MYM08, Sey12, YM97, dLHD10, KOT+00, TMM03]. **Compton** [KS77, OE17, ÖEO23, VG22]. **Computation** [BR65, CTS04, Nic10, RGFC13, EÜSB21]. **Computational** [BBB10, Duc97, LDP+04, Mar08b, NAY+08, OO05, RRMAF08, ST17, San98, SBK15, Tur07, LSZ+97b]. **computationally** [Wen21]. **Computations** [AH19b, Ano04l, Har18, LBV01, MRS+99]. **Computer** [FMA08, GBPSR10, MFMCN01]. **Computer-Algebraic** [FMA08]. **Computing** [Bis19, BPK23]. **Concentrated** [FIK+03]. **concept** [JJ20]. **Concepts** [GDL98, SCT15, SCT16, vL03]. **Conceptual** [Kar08]. **concerted**

[Hes22]. **Concluding** [Uda97]. **Condensate** [DB01]. **Condensed** [Ber03, Kar97, TMN10]. **Condition** [CCC17]. **Conditions** [KNN17, Bel22]. **Condon** [AHPD+03, AHPD+03, Pal04, SP99]. **conduction** [JJ20]. **Conductive** [TY85]. **Conductors** [KTMA08, Oni15]. **Conference** [Ano97a]. **Configuration** [ATL+18, AA03, Bel19, Bun18, EEL96, EM17, GC92, LHL18, RMMP17, RP18, RT18, SS99, CAG+21, SKS+19, WLM23]. **Configurations** [MFLK11, WD70]. **Confined** [Aqu09, Bad09, BC09, CTO18, CKC09, CLK15, DO09, GV09, GVFG09, Lau09, LK09, MFLK11, PV09, SPM09, SCM09, SBC09b, SBC09a, WD22]. **Confinement** [Cru09c, LKD05, BLC23, MBAPS19]. **Confirming** [Fuk15]. **Conformation** [HZ89]. **Conformational** [HSR98, Pul77]. **conformations** [GC01]. **Conformers** [SDGW98]. **Conical** [Pet98]. **Conical-Intersection** [Pet98]. **Conjugate** [Gos02b]. **Conjugated** [Nal09, RPSB00, SD04, TY85]. **Conjugation** [SS03]. **Conjunction** [Ano08h, ILS08]. **connected** [TM21]. **Connection** [AdMB99, BVHK03, Gut06, MC10, NFW+98]. **Conoidal** [LK09]. **conscious** [Per20]. **Consequences** [Coo18]. **Considerations** [Mar08a, MG20]. **Consistency** [DDPC95, Per90]. **Consistent** [DKMP98, GDL14, Sla72, VWP+98, WD70, LJKH13, LSC19, Ort22]. **Constant** [Nal00, SS22]. **Constants** [DE05, Gon98, Kar08, LvWH+01, Moh98, RM04, SPAS05]. **Constrained** [GM17, Lev90, DAB+23, Zap01]. **Constrained-Search** [Lev90]. **Constructed** [SW98]. **Construction** [KS97b, SO19c]. **Contact** [MFCT15]. **contacts** [MOB+03]. **Contemporary** [Sla81]. **Contents** [Ano67b, Ano68b, Ano70b, Ano72b, Ano73b, Ano74a, Ano75a, Ano77a, Ano78a, Ano80a, Ano81a, Ano81b, Ano82a, Ano82b, Ano85a, Ano98b, Ano98c, Ano01a, Ano01b, Ano01c, Ano03b, Ano03c, Ano04b, Ano04c, Ano04d, Ano05a, Ano05b, Ano05c, Ano06a, Ano07a, Ano08a]. **continuous** [NBS10, NBS12]. **Continuum** [ABC+98, BRL13, Cam12, JGCRC16, Jør74, KGW98, LJKH13, MFA21, Nic17, OOSS17, TS10, CTSSO19]. **Contracted** [VTPR97, VdLCPT98]. **Contribution** [MYM08, ST07, JMWG19]. **Contributions** [FAS+98, OOSS17, Ram08, CTSSO19]. **Contributors** [Ano64b, Ano64d, Ano65b, Ano65d, Ano67c, Ano67e, Ano68c, Ano68e, Ano70c, Ano70e, Ano72c, Ano72e, Ano73c, Ano73e, Ano74c, Ano75c, Ano77b, Ano77d, Ano78c, Ano80b, Ano80e, Ano81c, Ano81d, Ano81i, Ano81j, Ano82e, Ano82c, Ano82d, Ano85b, Ano85c, Ano88b, Ano89b, Ano90a, Ano91a, Ano92a, Ano92b, Ano94b, Ano95a, Ano96a, Ano97b, Ano97c, Ano98g, Ano98h, Ano98i, Ano98f, Ano98d, Ano98e, Ano99b, Ano99c, Ano99d, Ano99e, Ano00a, Ano00b, Ano01d, Ano01e, Ano01g, Ano01f, Ano01h, Ano02, Ano03d, Ano03e, Ano03f, Ano04e, Ano04f, Ano04g, Ano05d, Ano05e, Ano05f, Ano06b, Ano07b, Ano08b, Ano08c, Ano08d, Ano09a, Ano09b, Ano09c, Ano10a, Ano10b, Ano11a, Ano11b, Ano12a, Ano12b, Ano13c, Ano14a, Ano15a, Ano15b, Ano16a, Ano17a, Ano17b, Ano17c, Ano18a]. **Contributors** [Ano19c, Ano19d, Ano19e, Ano20a, Ano20b, Ano21a, Ano21b, Ano22a, Ano22b, Ano23a, Ano23b, Ano24a, Hog13c, Hog18c, SB13b]. **Control**

[Kra99, ML18, MM99, CM24]. **Controlled** [ALND10, ST17]. **Conundrums** [Cal13]. **convection** [Nal23]. **Convergence** [Bas78, CÅ01, DDPC95, KMJ97, OB23, SW98, Sil14, VWP+98, BG23]. **convergent** [SÁ23a]. **Cooling** [Phi98]. **cooperation** [SBK+08]. **Cooperative** [Chi03, GWM+03, NP03]. **Coordinate** [Lev90, TAM04, DAB+23]. **Coordinates** [ACC99, Byl98, Har05, KO18, MFA21]. **Coordination** [Ber74]. **Copper** [HB14, MYW00, TP03, YFK+97]. **Copyright** [Ano64c, Ano65c, Ano67d, Ano68d, Ano70d, Ano72d, Ano73d, Ano74b, Ano75b, Ano77c, Ano78b, Ano80c, Ano81e, Ano81f, Ano82f, Ano82g, Ano85d, Ano86a, Ano88c, Ano89c, Ano90b, Ano91b, Ano92c, Ano92d, Ano94c, Ano95b, Ano96b, Ano97d, Ano97e, Ano98j, Ano98k, Ano98l, Ano99f, Ano99g, Ano99h, Ano08e, Ano08f, Ano09d, Ano09e, Ano09f, Ano10c, Ano10d, Ano11c, Ano11d, Ano12d, Ano12c, Ano13d, Ano14b, Ano15c, Ano15d, Ano16b, Ano17d, Ano17e, Ano17f, Ano18b, Ano19f, Ano19g, Ano19h, Ano20c, Ano20d, Ano21c, Ano21d, Ano22c, Ano22d, Ano23c, Ano23d, Ano24b, Hog13d, Hog18d, SB13c]. **Core** [CS04, FVB99, OTA97, PGV97, CCM+19, FB20, MKK+01]. **Core-and-Bond** [CS04]. **Core-electron** [PGV97]. **Core-Hole** [OTA97]. **Correct** [LRCR98, Bel22]. **Corrected** [JGCRC16, LBV01, LRCR98]. **Correction** [AHPD+03, Per90, Por04, LSC19, YNNU03]. **Corrections** [DKMP98, EM17, LT98, PEZB98, PSS98, SJO05, YZDM01, VG22]. **Correlated** [DBC17, HA13, Har17, Hät05, MS03, MS65, NA19, Ryc98, SBH+20, Sau05b, SS99, SM23, SA23b, SCJ+23, Tew21]. **Correlation** [AH19b, BŚG17, HS86, HB14, HM21, IL98, JSF08, Kap98, KB98, KD11, KvH99, LBV01, MW98, MP89, Nes98, She15, Sla72, ŚBG14, SCN03, SDGW98, UK05, VWP+98, HO16, ORL23, SO19c, VdLCPT98]. **Correlations** [DB01, DB13, Gre98, OYI+00, BFHS23, WD22]. **corresponding** [LPC24]. **Cosine** [AFE13]. **Cost** [GDL98]. **Cost-Effective** [GDL98]. **Coulomb** [Ave13, AA18, BH24, CCA13, DGA18, GAM+13, GW23, Har04, KO18, LT98, LPC24, LJ17, Rui23, Sil14, SSS05]. **Coulomb-Breit** [LT98]. **Coulombic** [KNN17]. **Coulson** [SPH14]. **Coupled** [BPK23, Cam12, CCSZ01, FP06, GEO91, HJ99, HS86, KB86, LEK01, Les75, LGJP99, MDBM98, MH98, MFCT15, MKB04, MMSK16, MSM17, PM16, PB99, RR05, RMMP17, SB99, WN05, BB21, CCM+19, EÜSB21, GPEB21, LMK19, MK23, TMK21, TM21, PJH05]. **Coupled-Channel** [Les75]. **Coupled-Cluster** [Cam12, FP06, HJ99, HS86, KB86, LEK01, MH98, PB99, SB99, WN05, BPK23, MKB04, EÜSB21, MK23, TMK21, TM21]. **Coupled-Cluster-Theory** [PM16]. **Coupling** [ÅVM96, BVHK03, Chi03, DE05, ERC88, Kry03, MRS+99, Nal00, PB05, RM04, SPAS05, BMR+24, JS21, SBC+03]. **Couplings** [CPBS05, Lon99, SPAS05, SKS+19]. **Cousins** [RK04]. **Covalency** [BFHS23, OYI+00]. **Covalent** [She15]. **CPMD** [PWZ+08]. **CPU** [LH20]. **Cr** [ADA03, IOA03]. **CrF** [MKK+01]. **Criterion** [Per17]. **Critical** [BB99b, CCC17, HK03, IKN+08, ZZ08]. **Cross**

[CTSDÖ04b, CTSDÖ04a, HMH+18, Jos08, LC03, PBK04, RGFC13, MG22]. **Cross-caps** [LC03]. **Cross-Sections** [PBK04]. **Crossing** [SH95]. **Crossover** [LPDB03, NeMM03]. **Crystal** [ADA03, Jan65, MYW00, KC19]. **Crystalline** [HOI+08]. **Crystals** [AAM04, ABGM03, BJV86, Chi03, GWM+03, Jan65, KSY08, YKY+00, IOA03]. **Cs** [BJMB14, BMPV99, APNM03, SSS05]. **CSCH** [SSS05]. **CSDA** [AGO07]. **CSDA-Ranges** [AGO07]. **Cu** [SMAS08, ARS99, FU00, Fuk03, KC19, Mam19, NHYU03, SHBC19, UJYU03, WHB+24, YNNU03]. **Cu-** [NHYU03]. **Cubic** [APNM03, AHPD+03, ABGM03, HJ99]. **Cuprate** [DB01]. **Cuprates** [Fuk15, Kri03]. **Current** [Del74, Har04, Kho04, OW08, SBSL08]. **Currents** [CPBS05, FTG22]. **Curve** [SH95]. **Curves** [HBT+00, MCM14, MMSK16, MSM17, LMK19, SM23, TMK21]. **cusp** [LSC19]. **Cyanide** [ARS99]. **Cycloadditions** [RGA99]. **cyclobutanone** [MFMCN01]. **Cyclodextrin** [DNM+14, RMN+14, dLHD10]. **Cyclohexenone** [GBHM14]. **Cylindrical** [LKD05]. **Cytosine** [MBM99].

D [BRW08, SRZE04]. **D'Alembert** [Per17]. **Dalton** [BND81]. **Damage** [BB13, BB15, CL07, Tur07, vS07, SS22]. **Damages** [ST07]. **Darwinian** [BP20]. **Darwinism** [Brä22]. **Data** [KS97b, OO05]. **Dawn** [KvH99]. **DC** [KGI+19, SD04, dLHD10]. **deactivation** [Dur20]. **Decades** [GMP98, KKK+97, Nor98]. **Decay** [AK12, Gre08, KS88, MTA00, RF13, TMMS10, UYT97]. **Decoherence** [MCP12]. **decomposing** [Hog23c]. **Decomposition** [MC10, PL98]. **Decoupling** [NSM11]. **Dedication** [Ano96c]. **Defects** [Kuk14, MAS03]. **Definition** [Yas23]. **Deformations** [Kuk14, SIY+19]. **Deformed** [KMR01]. **Degenerate** [SBDD03, AR03]. **Degrees** [Nal06]. **Degrees-of-Freedom** [Nal06]. **Del** [LSZ+99a]. **Delocalization** [MFCT15]. **Delocalizations** [LR72]. **Delocalized** [Nal09]. **Delocalized/Conjugated** [Nal09]. **Dense** [DTC04, SPAS05]. **Densities** [AAAC04, BLKS78, TM13]. **Density** [AdMB99, ARS17, BR05, BK70, Bro98a, Bro98b, BŚG17, CDBG00, CD05, Cio90, CS77, Cru09c, Dah01, DR90, EG99, EEL96, Fuk15, GW17, GDL98, GBHM14, Gon98, GL90, GK90, Har90, HBT+00, HL90, JGCRC16, Kho04, KMHL13, KS90, KB98, Kry81, LBV01, Lev90, LS03, LDNP99, Lon99, LSZT90, LSZ+98a, LK90, LLBK+98, MRS+99, MTS04, McW98, Mic99, MT04, MNR+98, Min22, MYM08, MOB+03, Nag97, Nal00, Nal03, Nes03, Noo09, Öhr02, Oli90, PKYM01, Per98a, Per90, PEZB98, PGP17, PL98, RPSB00, RTV05, RP72, SRZE04, SS90, ŚBG14, UJYU03, VKI97, VRG90, WT99, WmG18, Yan90, YZDM01, vL03, BSL+19, GTB23, VdLCPT98, Zap01]. **Density-Based** [WmG18, BSL+19]. **Density-Dependent** [ŚBG14]. **Density-Functional** [EG99, Lev90, LS03, SS90, Min22]. **Density-Gradient** [KS90, PEZB98]. **Density-Matrix** [PKYM01]. **Dependence** [CDK15, FPL97, GP14, HK03, HBKS03, Ono00, ZLL+20]. **Dependent** [ARS17, BBB10, GK90, HG17, JGCRC16, KMHL13, LHL18, Lin17c, Löw67c, MKN10, MCA+18, Öhr15, Öhr17, ŚBG14, VTM98, WT99, LSZ+99a,

LSZB00, NA19, PS21, WLM23]. **Deposition** [CTS04, CTSDÖ05, CTCS05, CMJR+04, MBO+07, Sab97, Mic22]. **Deprotonations** [LDP+04]. **Depurated** [MMM18]. **Derivation** [FMA08, LK90, WN05]. **Derivative** [BB21, BB22a, IL98, Per90]. **Derivatives** [Cam12, HJ88, LDB95, WN05]. **Derived** [AAAC04, ŚBG14]. **Described** [Cam12, YTC+05]. **describing** [Hog23c]. **Description** [ABC+98, HL97, HS86, Sla81, Sut01, WD70, Nal23]. **Descriptions** [FVB99]. **descriptors** [BSL+19]. **Design** [Oli12, Oni15]. **Detachment** [ZDZO11]. **Determinant** [ATL+18, CAG+21]. **Determination** [ASGG08, SOS13, SSV98, SKS+19]. **Determine** [Fuk00]. **Determined** [Eks98, SBF+08]. **Determining** [BWK97, KS88, LASV18, Sme99]. **Detonation** [PM14]. **Deuteration** [LGK+99]. **Deuterium** [LJK+08]. **Development** [BMPV99, LDP+04, Nik70, OW08, OO05, TMN10, LH20]. **Developments** [Ber74, EEL96, HBE64, I'H64, LLBK+98, Pet98, SS98, San98, Sid18, SGM+13, TAM04, CCT02]. **DFT** [ABGM03, AR03, CKC09, KT15, LS07, Mam19, PS21, SKGŚ23]. **DFTB** [dLHD10]. **DFTB/UFF** [dLHD10]. **DH** [BMR+24]. **Diabatic** [TA04, Tap09]. **Diagnosis** [BSL+19]. **Diagnostics** [BB11, BB21]. **Diagonal** [DB13]. **Diagrammatic** [PČ75]. **Diagrams** [Sal74, SH95, WP06]. **Diamagnetic** [CE72, CPBS05, Vis05]. **Diamide** [HSR98]. **Diamond** [MTS04]. **Diaqua** [MYW00]. **Diastereoselectivity** [RGA99]. **Diatomic** [BC80, IS01, KGW98, Kob97, KK85, MK18, OO05]. **Dibromo** [MYW00]. **dications** [SM22]. **Dichroism** [CE72, PR05]. **Dielectric** [HL90, MTS04, MM13, AA19, VG22]. **Difference** [IS01, QGW01]. **Different** [LvWH+01, PS05a, CCT02, WLM23]. **Differentiability** [LS03]. **Differential** [FH65, SGB16, Ber02]. **Differentiation** [NSM11]. **Diffraction** [CS77]. **Diffusion** [FIK+03, TAU17]. **Difluoride** [MYW00]. **Dihedral** [CLK15]. **Dihydrates** [HTS+00]. **Dilated** [MM96]. **Dimensional** [CCA13, KMR01, RA19, SPD09]. **Dimensionally** [FCH15]. **Dimensions** [Ros98]. **Dimer** [BHM17, MCG+08, ORL23, SCJ+23]. **Dimers** [BU97]. **Dimethyl** [Fuk08b]. **Dimethylamine** [SSV98]. **dioctyloxyphenyl** [YKY+00]. **Dioxide** [PM16]. **Dioximato** [YKY+00]. **Dipolar** [RGA99, SJO05]. **Dipole** [AB73, BO86, CTO18, CCM05, JMWG19, OOSS17, PS05a, RM04, CTSSO19, PS21]. **Dipole-bound** [JMWG19]. **Dirac** [BH24, Cru09c, Lin02, Öhr16, QGW01]. **Dirac-Weizsäcker** [Cru09c]. **Direct** [DDPC95, GDL14]. **Directly** [Sal74]. **Discontinuity** [CTO18, Per90]. **Discotic** [YKY+00]. **Discoveries** [Wyb97]. **Discrete** [EG99, OW08, SGB16, SYIY03]. **Discussion** [KT15]. **disorder** [OTA03]. **Disordered** [Kar97]. **Dispersion** [HJ99, VG22]. **Dissimilarity** [SNM+97]. **Dissipative** [Brä02, Mic22]. **Dissociating** [Sut01]. **Dissociation** [BWH08, BŚG17, Hog18e, BLC23]. **Dissociative** [SSS05]. **Distances** [TTLB04]. **Distorted** [Bel22, BRL13, LK13, RGFC13]. **Distortion** [ITI+00, Kat03]. **Distortions** [LM03]. **Distortivity** [Fow03]. **Distributed** [GW01, MW98, QGW01, WM97]. **Distribution** [BWK97, CTSO04, OE17].

Distributions [CS77, KS77, AP03]. **Disulfide** [PM16]. **divalent** [FB20]. **DNA** [AGO07, CL07, Coo18, FB20, JA07, Krs16, KN01, Lad73, LS07, Löw65c, SOS11, Sim07, vS07]. **Do** [SS17]. **Does** [Tak19]. **domains** [Tew21]. **Doped** [CY00, HDB03, SCN03, TP03, Hog21, IOA03, Ito03]. **Dosimetry** [PGJ07]. **Dots** [SPD09]. **Double** [MCM14, PLA01, Bel22, SM22]. **Double-Barrier** [PLA01]. **Doubles** [HS86, LGJP99]. **Doublets** [DeB09]. **downfolding** [BPK23]. **Driven** [BGG+07, SBH+20, WLM23]. **Droplets** [GNM08]. **Due** [FU00]. **Dunham** [OO05]. **During** [UYT97, MU03]. **DV** [Ada97b, Ada00, CL00, FSB+97, Fuk03, Fuk15, Gut97, IFAY08, Kaw97, KNM+08, LSZ+00, MYW00, MW08, MKK+00, Mur08, Nak00, NHYU03, OTA97, Ros97, SBA+03, SBK+08, SNMI00, Tan00, UMD08, YFK+97]. **DV-X** [Ada00, CL00, LSZ+00, MYW00, MKK+00, Nak00, SBK+08, SNMI00, Tan00]. **dye** [GTB23]. **dye-sensitized** [GTB23]. **Dyes** [BMPV99]. **Dynamic** [FAS+98, NeMM03]. **Dynamical** [AAM04, Brä04, CTSDÖ04a, NP03]. **Dynamically** [ILS08]. **Dynamics** [ACC99, BR82, BHV+00, BJV86, CTSDÖ04b, CMJR+04, DW98, För94, GMB04, HHK+98, HS19, HG17, HPRR10, HBGvM19, IBB+19, ILS08, JGNJ08, KD11, MCG+08, Mat96, Mic17, PWZ+08, RFG+98, Saa01, Sab97, SGM+13, TA04, dLHD10, GTB23, Mic02, Mic22, MFMCN01, NTT20, SBH+20, WLM23].

E-Hy-CI [RSP21]. **E-learning** [MP22]. **Early** [BB11]. **Earth** [KRL01, STO+00]. **Easy** [Col68]. **Eckart** [YTC+05]. **Economical** [BR65]. **Edaravone** [RMN+14]. **Edge** [KsKsN08, MYW00, OTA97, YFK+97, CCM+19, NHYU03]. **Edited** [Ano90c]. **Editorial** [Ano88d, Ano89d, Ano91c, Ano92e, Ano92f, Ano95c, Ano96d, Ano97f, Ano97g, Ano98m, Ano98n, Ano98o, Ano99i, Ano99j, Ano99k, Ano01i, Ano03g, Ano08g, Ano09g, Ano09h, Ano10e, Ano10f, Ano11e, Ano12e, Ano19i, Hog13e, Ano13e]. **Editors** [Ano82h, Ano94a, Ano98a, Ano08l, Ano08n, Ano09i, Ano09j, Ano10g, Ano10h, Ano11f, Ano11g, Ano12i]. **educated** [SÁ23a]. **educational** [Kar02]. **Effect** [ADA03, BP82, BO86, Chi03, FE97, GWM+03, GBPSR10, HBKS03, ITI+00, KT98, MCC03, NM00, NP03, OTA97, Por04, SKT+03, SCM09, Sjö04, SCN03, VWP+98, NA19, WHB+24]. **Effective** [CHSC03, GW18, GDL98, KKGG98, MMM18, Mic74, Nag01, MMM19, SKGŚ23]. **Effectiveness** [AFE13]. **Effects** [AB73, ABC+98, BMPV99, Bas64, BS04, Bic13, BB14, BŚG17, CTSDÖ05, CTO18, CHSC03, CC97, DKV+19, ERC88, Fuk00, GMLSC+10, GM17, GC01, GVFG09, IKN+08, Jør74, JGNJ08, KH03, KD11, KBS03, Laz04, LGK+99, OYI+00, Ono00, Pet98, PSAP10, PGN04, RM04, SIY+19, SDGW98, TS10, UK05, WDD16, AA19, Kar24, SS22, VdLCPT98]. **Effects-Selected** [CHSC03]. **Efficient** [PTBH13, BG23, KBH23]. **Eigenfunctions** [Sal74]. **Eigenstates** [RP72]. **Eigenvalue** [YTF78, Gos02b]. **Eight** [LPC24]. **Einstein** [McW99]. **Ejection** [Sim99]. **Eka** [LvWH+01].

Eka-Lead [LvWH+01]. **Elastic** [HHU+21, SJAB+22]. **Electric** [FPL97, IS01, KGI+19, LDB95, Laz04, LHL18, SJO05, UK05, YÖ13]. **electrical** [BLC23]. **electrode** [KTA03, SYIY03]. **Electrodes** [OBHM17, KTA03]. **electrodynamic** [PMK23]. **Electrodynamics** [MDÖ05, Moh98, Sal11, Sau05a, SBG+98, SAL10, SGK+08]. **Electromagnetic** [BGG+07, IBB+19]. **Electron** [Ada00, AGO07, AYÖ17, Ave98, Ave13, BGG+07, BL18, BS72, BC80, CTSDÖ04b, CO17, DBC+99, DSR81, FH65, FJS+04, Gal73, HHK+98, HUS+11, HPU+17, HMH+18, HS05, HSS+04, HS86, HB14, HO16, HM21, Hyl64, JA07, KS88, Kap98, Kle77, KDG97, KD11, KvH99, LT98, LJ17, LK13, LR72, Lon99, Lyk64, MLPD+98, MM96, MA04, MTA00, MSM17, NA04, Nes75, Nic17, NM03, OYI+00, OM03, Ohn67, ÖB81, Ort99, PKYM01, RP72, RLF17, Sab97, Sal74, STZY18, SPM09, Sim99, Sim05, SHBC19, SSS05, SGK+08, SS04, SGM+13, SCN03, SDGW98, TM13, UK05, Yea05, ZDZO11, ZP17, AO03, AP03, Bel19, Bel21, Cru09c, FCAG19, GTB23, GPEB21, IOA03, Lar02, LSC19, MOB+03, MU03, Ort22, PGV97, Rou20, SBH+20, SPD09, WLM23]. **Electron-** [NM03]. **Electron-Capture** [MTA00, Bel21]. **Electron-Driven** [BGG+07]. **Electron-Impact** [HMH+18]. **Electron-Ion** [LJ17]. **Electron-Nuclear** [CTSDÖ04b]. **electron-nucleus** [LSC19]. **Electron-Pair** [TM13]. **Electron-phonon** [SHBC19]. **electron-positron** [AP03]. **electron-propagator** [Ort22]. **Electronegativity** [OPPZ06]. **Electronic** [Ada97a, ADRAB16, AB73, AH19b, AR03, AK12, BVHK03, Bas64, Bas78, BS04, BJMB14, BWK97, Bra67, CTO22, CD05, CMDN89, CCCC15, CY00, CL00, CCL03, CSZ99, Dau64, DO09, DA14, DB01, DB13, DBC17, EGCL91, EOH03, FP06, FCH15, FE97, Fuk00, Fuk15, GTB23, GSTvE98, GM91, GVFG09, Har18, HJ88, HOI+08, HTS+00, Hog13g, Hog14, Ito03, Jan97, KM98, KIT+08, Ker82, KIHA97, KNI+08, KC19, Kot68, Köv08, KE97, KE00, KTA03, Kuk14, LM97, Lin17a, LSZ+97a, MC10, MTS04, Mic99, MKH+97, MYM08, MMSK16, NIO03, Nal03, Nal06, Nal23, OTA03, PR05, PB75, PB99, PP68, RPSB00, SS98, Sal74, ST78, SNM+97, Shi12, SNIM08, SMAS08, TY85, Tap01, TA04, Tap09, YKS+12, YM00, AO03, BSL+19, KOT+00, LSZ+99a, LSZB00, MMM22]. **electronic** [SCE19, SKS+19, YIYM03]. **Electronically** [MT04]. **Electrons** [ACDK72, BG73, FVB99, She15, Sim07, Suc98, ST07, AA19, NBA20, SJAB+22, SM23]. **Electronuclear** [TA04]. **Electrostatic** [Jør74, PTBH13, ST78, FSP23, ŻMM23]. **Element** [AAE+01, BS05a, Fuk15, SGB16]. **Elemental** [ASGG08]. **Elementary** [CDP82, Gre08, MCG+08]. **Elements** [CD05, KE98, KRL01, MTA00, RP72, Bar23, TMM03]. **Elliptic** [PS05b]. **Elpasolites** [APNM03]. **Elucidation** [Oni15, SIY+19]. **Embedded** [KE97, KE00]. **Embedding** [LC03, LJKH13, OK11, MG21]. **Emerald** [IOI+00, ITI+00]. **Emission** [JGCRC16, Kaw97, MKK+00, MTA97, SS04, Uda00, UMD08, Mur03]. **Emitted** [AVB08]. **Emitters** [BWVD+13]. **Empirical** [BRL13, HSS+04].

Employing [FP06, Kou15]. **Encaged** [Dol09]. **encoded** [BB22a]. **Endo** [RGA99]. **Endo/Exo** [RGA99]. **Endohedral** [CTO18]. **Energetic** [AGMdV+13, Ber14, CHR13, Kuk14, MF14, PGJ07, Sab14a, TR14]. **Energetics** [LYM03, PL98]. **Energies** [AGO07, Gal73, HMH+18, HL90, JSF08, LM03, PEZB98, PGP17, RR05, SOS11, SYM+08, VI01, ZDZO11, Bel22, CTSSO19, CTO22, CTC22, MKK+01, Ort22, PEMC23, SSO19, TBM01]. **Energy** [AJ04, Apo01, AL04, BB99b, Ber14, Bic13, LJK+08, Bun18, CTS04, CTSDÖ05, CTCS05, CMDN89, CMJR+04, CMVPFC16, DKMP98, DDPC95, GP91, GC92, Glu19, GS04b, HBT+00, HL90, IL98, Kho04, KSY08, KB98, Köv08, LBH+17, LJ17, Les75, LDNP99, LASV18, Mic22, MW98, MF04, MM13, MBO+07, MCM14, MMSK16, MSM17, Nak00, Nes75, Oli12, Per98a, PB14, PLA01, RGFC13, Sab97, SOS13, SPD09, SJO05, SOS15, SW98, Sim07, Sla64, SSS05, TMN10, Tők19, WN05, YZDM01, Bun23, GG20, Kar24, Lar02, LMK19, NA19, PGV97, SH19, SM23, TMK21, ŻM23]. **Engels** [Miy03]. **Engineering** [DO09]. **Enhance** [PB14]. **Enhancement** [LASV18]. **Enlarge** [MRS+99]. **Ensemble** [PGP17]. **Ensembles** [CDK15]. **Entanglement** [KO19]. **Entropy** [Kou15, Brä22]. **envelopes** [BB22a]. **Environment** [GBPSR10]. **EOMXCC** [PB99]. **EPR** [Coo18, TP03]. **equal** [NBA20]. **Equalization** [OPPZ06]. **Equation** [Löw85c, Löw98, MFCT15, MKN10, MKB04, Öhr16, QGW01, VTPR97, WN05, Yas17, BG23, BH24, ORL23, Yas23]. **Equation-of-Motion** [WN05, MKB04]. **Equations** [BE01, BS05a, Cal85, Kob97, LK90, Per17, SGB16, SKGŚ23, VdLCPT98]. **Equilibria** [KZR86]. **Equilibrium** [Spe78]. **Equivalence** [EBR92]. **Error** [Bun18, VWP+98]. **Errors** [KB98, Bun23]. **Estimating** [Apo01]. **Estimation** [Sey12, SIY+19]. **Ethanedione** [YKY+00]. **Ether** [Fuk08b]. **ethylene** [RZTSW23]. **ETOs** [AFE13]. **ETS** [ŻMM23]. **ETS-NOCV** [ŻMM23]. **Euristic** [ST78]. **eV** [AGO07, HHU+21, Sim07, WHB+24]. **Evaluating** [Hog18e]. **Evaluation** [AYÖ17, CB92, KS77, KNM+08, ÖÖ13, SB99, ALA23, BSL+19, MKK+01, Rui23]. **Even** [KGW98]. **Even-Tempered** [KGW98]. **Evolution** [Brä19, Löw67c, Tos08]. **Evolving** [SIY+15, SIY+19]. **Exact** [Bel06, BC09, DeB09, GC10, KB98, Kob97, KNN17, MRHdCK15, Ort99, SPM09, vL03]. **examined** [MG22]. **Examining** [Brä12]. **Example** [Lyo08, MCM14]. **Exchange** [Jan65, KB98, LRCR98, LDNP99, MRHdCK15, MF04, Sla72, ŚBG14, SCTH+07, Bel22, JS21, ORL23, SO19c]. **Exchange-Correlation** [Sla72, ŚBG14, ORL23, SO19c]. **Exchange-Energy** [LDNP99]. **Exchanges** [PLA01]. **Excitation** [ATL+18, Bel09, BLKS78, GP04, LM03, PGP17, RR05, SOS13, SOS11, SOS15, Tak19, AGS+19, CTSSO19, CTO22, CTC22, FCAG19, GJP23, Lar02, MKK+01, SSO19]. **Excitations** [FLV99, Kuk14, CCM+19, SCE19]. **Excited** [AB73, Hät05, HBKS03, KM98, LKD05, MT04, Nag97, Nag01, Oli90, PB99, RM04, Sme99, WN05, Dur20, MK23, Nag03, OB23, PS21, SZP21]. **Excited-State** [AB73, WN05, Dur20]. **exciton** [GJP23]. **existing** [BPK23].

Exo [RGA99]. **Exotic** [Ano08h]. **Expansion** [BR65, MKN10, MP89, Sil14, CAP19]. **Expansions** [AA01, FP06, FMA08, KS90, SPH14, Sid18, SCJ+23]. **Experiment** [RC05, VWOS89, PMK23]. **Experimental** [ASGG08, BKC68, BLKS78, LGK+99, Miy03, RAR+08, ZBM98, Hog14]. **Experimentalist** [vS07]. **Experimentation** [LDP+04]. **Experiments** [Ano08h]. **Explicit** [Vis05, SS22]. **Explicitly** [Ryc98, SA23b, SCJ+23, Tew21, TM21]. **Exploding** [LJ17]. **exploration** [PB20a]. **Explored** [ABGM03]. **Exploring** [ORL23, WLM23]. **Exponential** [AA15, CB92, FP06, Hog13g, HM21, Nik70, ZP17]. **Exponential-Type** [AA15]. **Exponentially** [Har17]. **Expression** [PTBH13, SYM+08, Yas17]. **Expressions** [Vis05, TM21]. **Extended** [BC00, Cal85, CDBG00, DB01, FP06, LK90, May80, Mon05, Uda00, Min22, Ort22]. **extended-Koopmans-theorem** [Ort22]. **Extending** [BBB10]. **Extension** [GVFR98, Lev14, RP18]. **Extensive** [LJK+08]. **Extensivity** [EM17, SB99]. **External** [SD04, TA04, NA19]. **extremely** [MG21].

F [Kom05, CTSSO19, CCM05, UYT97]. **F12** [Tew21]. **Facility** [Ano08j]. **Factor** [LASV18]. **Factors** [AHPD+03, SJO05]. **failure** [Sak03b]. **Family** [DLMS03, VT24]. **Far** [Eks98]. **Fast** [Ave13, Bel06, Bel09, BMM13, DeB09, LK13, SS04, Bel21]. **Faults** [FU00, UJYU03]. **Favorite** [FCC04]. **Fe** [CSZ99, ARS99, YNNU03]. **Fears** [Sut98]. **Features** [Kry03, Lin17a]. **Fermi** [Cru09c, CTC22, MYM08, SO19c]. **Fermion** [Per98a, LSZT90, PČ75]. **Ferroelectricity** [IKN+08]. **Feshbach** [SW81]. **Few** [Har04, KO19, LT98, Mic17, Shi12, Mic02]. **Few-Atom** [Mic17, Mic02]. **Few-Body** [Har04, KO19, Shi12]. **Few-Electron** [LT98]. **Feynman** [FMA08, GM91]. **Field** [BVHK03, FPL97, FSB+97, Glu19, GDL14, HG17, HPRR10, IBB+19, JH99, Kob68, KGI+19, Laz04, LJKH13, Nic10, Nic17, Per98a, PLA01, Sla72, WD70, EÜSB21, NA19, Ort22]. **Field-Assisted** [PLA01]. **Field-Free** [Nic10]. **Field-Induced** [Nic10, Nic17]. **Fields** [AAM04, DSW04, Gre08, IS01, SBG+98, SD04, TA04, VRG90, BB22a]. **Fifth** [KB86]. **Fifth-Order** [KB86]. **Fifty** [Cra99]. **film** [KBH23]. **Films** [KsKsN08]. **Finite** [AAE+01, BS05a, DR90, Fuk15, IS01, KCM70, OOSS17, QGW01, SGB16, WDD16, SKGŚ23]. **Finite-Difference** [IS01]. **Finite-Element** [AAE+01, BS05a, SGB16]. **First** [Ada97b, CHR13, DA14, Fuk08a, Fuk08b, HPRR10, HBGvM19, IOI+00, KIT+08, KSY08, KG12, MTS04, MCC03, OYI+00, PM16, Sak03a, WN05, Yam03, YKC+08, KTA03, VdLCPT98]. **First-order** [MCC03]. **First-Principle** [HPRR10]. **First-Principles** [Ada97b, DA14, Fuk08a, Fuk08b, HBGvM19, IOI+00, KIT+08, KSY08, MTS04, OYI+00, YKC+08, Sak03a]. **Fischer** [CL05]. **Fission** [BHM17, SKS+19]. **Fitted** [MRHdCK15]. **Five** [VT24]. **Floquet** [LMSP01, Pal04]. **Fluctuation** [Jeh65]. **Fluids** [CCCC15]. **Fluorescence**

[HBE+98]. **Fluoride** [UMD08]. **Fluorides** [TSON00]. **Fluorine** [SPAS05]. **Fluorine-Fluorine** [SPAS05]. **Fock** [BB99b, DKMP98, OE17, ÖEO23, BGW73, CBSM20, DAB+23, FCH15, GV09, GW23, Hur73, HMC73, LBV01, LEK01, LMK19, LFM89, LM92, May80, MMM18, MK18, MMSK16, Nes67, Sme99, TMK21]. **Fock-Space** [LEK01]. **folding** [LL20]. **Following** [AGS+19]. **footing** [NBA20]. **Force** [DSW04, Gon98, Krs16, PTLGOM12, Suc98, TTLB04, EÜSB21]. **Forces** [Kap98, LR72, MS67, Sal11, ST78]. **Forcing** [KSG08]. **Foreword** [Ano08i, Köv97]. **Formal** [Noo09]. **Formalism** [BMP03, CS04, Cru09c, GM91, Löw85c, MM13, OO05]. **Format** [Ano88a, Ano89a, Löw88a]. **Formation** [KV08, MCG+08, BMR+24, JMWG19]. **Forming** [ST17]. **Formulae** [SIY+19, Wyb97]. **Formulas** [ZP17]. **Formulation** [Lev90, MDÖ05, Yan90]. **Formulations** [MDBM98]. **formyl** [HDFT24]. **Foundation** [Brä19]. **Foundations** [CO17, Hal91, LK90, MG21]. **Four** [BMR+24, BL18, BMM13, GMP98, Har05, HA13, Har17, MYW00, Nor98, QSG98, RLF17, BMC97]. **Four-Body** [BMM13, Har05, HA13, Har17]. **Four-Electron** [BL18, RLF17]. **four-membered** [BMC97]. **Fourier** [AYÖ17, FCH15, Mon05, ÖÖ13]. **Fr** [BJMB14]. **Fractionation** [Lyo08, Mar08a]. **Fragmentation** [SCTH+07, ST07]. **Fragments** [GVFR98, ZDZO11]. **Frame** [YTC+05]. **Framework** [ATL+18, CCVB94, Gut97, LJKH13, Tap17, LT21, SKGŚ23]. **Franck** [AHPD+03, Pal04, SP99]. **Frank** [KT15, Ano03h, Kai15, SCT15, SCT16]. **Free** [KT15, Mat64, MFLK11, Nic10, TMN10, VKI97, vS07, GG20]. **Free-Energy** [TMN10]. **Free-Radical-Induced** [vS07]. **Freedom** [Nal06]. **Freeon** [Mat96]. **Frequencies** [BLKS78]. **Frequency** [MCP12, ML18]. **Friction** [TTLB04, BMR+24]. **Friend** [Lin99, OB22a, Öhr05]. **Froissart** [DeB09]. **Front** [Ano19j]. **frontier** [PEMC23]. **frustrated** [SPG+22]. **Full** [BE01, HS86, SED+98]. **Fullerene** [CKC09, KOT+00]. **Fullerene-like** [CKC09]. **Fullerenes** [CPBS05, Dol09, HDB03, Kat03, ZDZO11]. **Fully** [Bun23, CTG98, HA13]. **Function** [BMP03, DDPC95, FP06, KD11, MTS04, EW03]. **Functional** [ARS17, Bro98a, Bro98b, BŚG17, Cio90, Cru09c, DR90, EG99, EEL96, Fuk15, GW17, GDL98, GBHM14, Gon98, GL90, GK90, Har90, HBT+00, HL90, IL98, JGCRC16, KMHL13, KB98, LBV01, LRCR98, Len68, Lev90, LS03, LK90, LLBK+98, MRS+99, Mez96, MNR+98, Nag97, Nal03, Nes03, Noo09, Oli90, Oni12, Per98a, Per90, PGP17, PL98, RTV05, Rou20, SRZE04, SS90, VKI97, VRG90, WT99, Yan90, YZDM01, vL03, GTB23, LSZT90, LSZ+98a, MGAUP23, Min22, MPU19, MOB+03, Zap01]. **Functionals** [AdMB99, GP91, KB98, LDNP99, Löw96b, MRHdCK15, Nal00, vL03]. **Functioning** [KN01]. **Functions** [AFE13, BL18, BS05a, Bis67, BR65, BC00, BC09, CDBG00, CD05, CTG98, Dah01, Dau64, DGA18, FU00, GAM+13, GM17, Gil94, Har17, Har18, HPB17, KO18, Kla81, KNN17, LV90, Lev14, McG04, MS65, MFA21, Nes03,

PS05a, PS05b, RMMP17, Ryc98, SJO05, SW98, SPH14, SNIM08, ZP17, ALA21, ALA23, LPC24, Per20, SA23b, TM21, VT24, VG22, Wen21]. **Fundamental** [DE05, GM05, Moh98, QSW20, SBF+08]. **Fundamentals** [GM17, MNR+98, Spe78]. **Further** [AFE13, TAM04, MG21]. **Future** [HKS90, OW08].

GaAs [Ito03]. **Gallium** [KSY08]. **Gap** [Cal85, IFAY08, SS90]. **Gaps** [Kri03]. **Gas** [BG73, HSR98, Jan65, MRS+99, NA04, RAR+08, HM19]. **Gas-Phase** [HSR98, MRS+99, RAR+08]. **Gaseous** [ASGG08]. **Gauge** [Woo98]. **Gaussian** [ALA21, BL18, DR90, Gil94, GW01, HO16, HPB17, KGW98, MW98, PTC+13, QGW01, SW98, SA23b, WM97]. **Gaussian-Type** [DR90, SW98, ALA21]. **Geminal** [Wei04]. **Genealogical** [Sal74]. **General** [Brä08, CMDN89, Kry03, KNN17, LM92, LH20, Löw88b]. **Generalizations** [OPPZ06]. **Generalized** [AAG03, AAAC04, AA05, BLKS78, CTSOS99, FP06, GAM+13, GJP23, HW01, I'H64, Mic15, MFA21, SED+98, TA04, Tap09, Gos02b]. **Generated** [PTBH13, Sal74]. **Generation** [AAM04]. **Generator** [TAM04, DAB+23]. **Genetics** [Löw65c]. **Gentleman** [SO19b]. **GeO** [GP14]. **Geometric** [Nal06, PB14]. **Geometrical** [HJ88, LDB95, SIY+19]. **Geometry** [BHM17]. **GeV** [HHU+21]. **Giuseppe** [LSZ+99a]. **Giving** [PTBH13]. **Glance** [KG12]. **Glasses** [KE97, KE00]. **Glassy** [MKK+00]. **Glycine** [SOS11]. **Gold** [BHV+00, RK04, MOB+03]. **Goldstone** [FMA08]. **Good** [Cra99, QSG98]. **Goscinski** [Ano04i, SBK04]. **Got** [SS17]. **GPCR** [ST17]. **Gradient** [FPL97, KS90, Laz04, LRCR98, PEZB98, SED+98, YZDM01]. **Gradient-Corrected** [LRCR98]. **Gradients** [GC92, WN05]. **Grain** [Sak03b, OTA03]. **Grand** [CDK15]. **Graph** [Gut06, JH99, LC03, Yan81]. **Graphical** [LHL18]. **Graphite** [UMD08, KOT+00]. **graphitic** [Mur03]. **graphitic-structured** [Mur03]. **Green** [BMP03, BC00, KD11, McG04]. **Green's** [DDPC95]. **Green's-Function** [DDPC95]. **Ground** [CMVPFC16, KM98, KT15, LPDB03, MS03, MW98, RM04, RT18, Bel19, Hog21, MK23]. **Ground-State** [KT15, Hog21]. **Group** [Col68, DSR81, LHL18, LB92, Mat78, RPSB00, Sme92]. **Groups** [DSW04, Gal73, KCM70, Mez96, Ray95, Ser74]. **GSI** [Ano08j]. **GTOs** [ALA23]. **Guesses** [Wyb97]. **Guide** [Öhr16, ZLC+10]. **GW** [Mon05].

H [AGS+19, BRW08, CSZ99, DLMS03, HOI+08, Miy03, NeMM03, YKS+12, CLK15, Hog18e, Hog21, LK14, MBAPS19, Sau05b, SH19, SSS05, SS04, SEL01, TM13, YIYM03]. **H-Bonding** [LK14]. **Hadron** [Pau13]. **Hadrontherapy** [Fra13]. **Hafnium** [KsKsN08]. **Haldane** [IFAY08]. **Half** [BB99a, Sme99]. **Halide** [Tak19]. **Halides** [Jan65, LF09]. **Halo** [DY08]. **halogen** [GC01]. **Halogens** [ASGG08]. **Ham** [Ano03h]. **Hamiltonian** [CHSC03, FTG22, LEK01, Löw85c, Löw88b, LFM89, Mic74, Öhr16, YZDM01]. **Harmonic** [AAM04, KMR01, LKD05, VTM98]. **harmonically** [WD22]. **Harmonics** [AYÖ17, AA01, AA15, CCA13, MFLK15, SR73]. **Harris**

[Kai15, SCT15, SCT16]. **Hartree** [BGW73, CBSM20, DAB+23, DKMP98, FCH15, GV09, GW23, Hur73, HMC73, LBV01, LFM89, LM92, May80, MMM18, MK18, Nes67, OE17, ÖEO23, Sme99]. **HBXYBH** [BMC97]. **He-like** [BH24, VT24]. **Heat** [MYM08]. **Heavy** [Ano08h, Bic13, KE98, NA04, RGFC13, Bar23, MKK+01, MMM22]. **HeH** [CLK15, SJO05]. **Heights** [PEZB98]. **helical** [Min22]. **helices** [GG20]. **Helium** [Aqu09, GV09, GW18, Kob68, KMJ97, PV09, SCJ+23, VT24]. **Helmholtz** [BS05a]. **Heme** [Kot68]. **Heredity** [Löw65c]. **Heterostructures** [Kra99]. **HF** [Kob97, MCM14, PS05a, Sau05b]. **Hg** [HHU+21]. **HgI** [BKC68]. **Hierarchical** [SPG+22]. **High** [AAM04, BB11, BB17, BS05a, LJK+08, Bor03, DTC04, DB01, DB13, DBC17, Hug98, KE98, Köv08, MF14, MM13, RGFC13, RSP21, San98, SPH14, SGK+08, Sva98, VTM98, Bel22, BB22a, Sak03b]. **High-** [SGK+08]. **High-Accuracy** [KE98]. **High-Energy** [Köv08, MM13, RGFC13]. **High-Order** [AAM04, BS05a, VTM98]. **High-Power** [Sva98]. **High-Precision** [LJK+08, RSP21, San98]. **High-Resolution** [BB11, BB17]. **High-T** [DB01]. **High-Temperature** [DB13, DBC17]. **Higher** [BB14, KNN17]. **Higher-Order** [KNN17]. **Highly** [Ano08h, Ano08j, HS05, LT98, Ram98, SS99, ŚBG14]. **HITRAP** [Ano08j]. **Hole** [NM03, OTA97, SS03, GJP23]. **Homogeneous** [LDNP99]. **homotopy** [JJ20]. **honor** [LSZ+99a]. **Honour** [SBK04]. **Hopes** [Sut98]. **Hot** [DTC04]. **Hubbard** [DAB+23, DB01, ORL23]. **Hückel** [BE04, I'H64]. **Hunches** [Wyb97]. **Hund** [KP77]. **Hy** [RSP21, RSP21]. **Hy-CI** [RSP21]. **Hybrid** [ATL+18, GMB04, MRHdCK15, EW03, Rui23]. **Hybridization** [BB99a]. **Hydrate** [HBT+00, MYW00, PWZ+08]. **Hydrates** [KKK+97, PWZ+08]. **Hydrazine** [RNL14]. **hydride** [CBSM20, YIYM03]. **Hydrides** [SKT+08, SYM+08]. **Hydrocarbon** [Bro98a, Bro98b, LF09]. **Hydrocarbons** [KH03, ZZ08]. **Hydrogen** [Aqu09, LJK+08, Bra67, CTO18, CLK15, DE05, EGCL91, FRM70, FCC04, FJS+04, GAI08, KO18, Kom05, KMJ97, Krs16, Lau09, LK09, LKD05, MC10, MFLK11, MW98, OOSS17, PV09, PWZ+08, SIY+15, YM97, YM00, Fuk03, Hog23c, HDFT24, JS21, KBH23, PMK23, SZP21, WLM23, YIYM03]. **Hydrogen-Antihydrogen** [FJS+04]. **Hydrogen-Atom** [KO18]. **Hydrogen-Bonded** [FCC04, GAI08]. **Hydrogen-Bonding** [MC10, PWZ+08]. **Hydrogen-like** [Lau09]. **Hydroxy** [SDGW98]. **Hylleraas** [Har05, Har18, Rui23]. **Hylleraas-CI** [Har18, Rui23]. **Hyperbolic** [AFE13, MFCT15]. **Hyperfine** [Bli65, EEL96, GMP98, Lon99]. **Hypergeometric** [CAP19]. **Hypergolic** [RNL14]. **Hyperguinones** [Mam19]. **Hypermatter** [Gre08]. **Hyperpolarizabilities** [HJ99, LÅJM95]. **Hyperquantization** [ACDV01]. **Hypershieldings** [LDB95]. **Hyperspherical** [ACC99, ACDV01, AA01, AA15, CCA13]. **hyperthermal** [HM19].

Icosahedral [JL03, LC03, SBDD03]. **Ignition** [RNL14]. **II**

[YKY+00, BGW73, LFM89, LSZ+98c, MYW00, NBS12, SIY+15, SIY+19, TP03, YFK+97]. **III** [BG73, NeMM03, PM16]. **Illustrations** [JH99]. **Imaging** [BWVD+13]. **Impact** [ARS17, HUS+11, HPU+17, HMH+18, Heh18, KSG08, LJ17, SS04, ST07, MG22]. **Impenetrable** [Lau09]. **Implementation** [CTCS05, PM16, SGM+13, LH20]. **Implementing** [TL10]. **Implications** [Brä12, JGNJ08]. **Implicit** [SS22]. **Importance** [LK90, AO03]. **Important** [BRW08]. **Improve** [PEZB98]. **Improvements** [AFE13]. **Impurities** [FE97, Fuk00]. **Impurity** [KNI+08, MFCT15]. **Including** [KT98, CTO22, WHB+24]. **Inclusion** [MKB04, dLHD10]. **Incorporating** [MKK+00]. **Independence** [Kla81]. **Independent** [BBB10, BGW73, BG73, Gre73, Lyo08, Mar08a, PČ75]. **Index** [Ano64a, Ano64e, Ano65a, Ano65e, Ano67a, Ano67f, Ano68a, Ano68f, Ano70a, Ano70f, Ano72a, Ano72f, Ano73a, Ano73f, Ano74d, Ano75d, Ano77e, Ano78d, Ano80d, Ano81g, Ano81h, Ano82i, Ano82j, Ano85e, Ano86b, Ano88e, Ano89e, Ano90d, Ano91d, Ano92g, Ano92h, Ano94d, Ano95d, Ano96e, Ano97h, Ano97i, Ano98p, Ano98q, Ano98r, Ano98s, Ano99l, Ano99m, Ano99n, Ano00c, Ano00d, Ano01j, Ano01k, Ano04h, Ano08m, Ano12f, Ano12j, Ano13f, Ano13g, Ano13h, Ano14c, Ano14d, Ano15e, Ano15f, Ano16c, Ano17g, Ano17h, Ano17i, Ano18c, Ano19k, Ano19l, Ano19m, Ano20e, Ano20f, Ano21e, Ano21f, Ano22e, Ano22f, Ano23e, Ano23f, Ano24c, Apo01, Nak00, San92]. **Indices** [MNR+98]. **Indirect** [SPAS05]. **INDO** [BMPV99]. **Induced** [BGG+07, BWVD+13, BR17, KS88, Kho04, Nic10, Nic17, Sal11, Sim99, SS04, TS10, Uda00, vS07, HDB03, Yam03]. **Industrial** [Hog18e, SBK+08]. **Inelastic** [AGMdV+13, BR17, FCAG19, MM13, RGFC13, AMAA22]. **Inference** [Kou15]. **Infinite** [Kla81, Bar23, LK09]. **infinite-order** [Bar23]. **Influence** [PGJ07, FB20, Kar02]. **Influenced** [SSS05]. **Influences** [Jør74]. **Information** [Nal03, Shi12, Nal23]. **Information-Theoretic** [Nal03, Nal23]. **Informed** [TR14]. **infrared** [EÜSB21]. **Ingvar** [Nor98]. **Initial** [Gre73]. **Initiated** [RAR+08]. **Initio** [BŚG14, CL07, CH03, DRV82, DO09, DSW04, HPRR10, ILS08, Jan97, JcH18, KNI+08, KTC01, LBH+17, MBM99, PR05, PWZ+08, QSG98, RNL14, RFG+98, Sau05b, HO16, IKN+08, SM23, ŚBG14, ZDZO11, CG80, Chr72, MWL+05, San92, BMC97, Kap98, SSV98]. **Inlet** [SIY+15]. **Inner** [HUS+11, HMH+18, HL97, MU03]. **Inner-Shell** [HUS+11, HL97, MU03]. **Inorganic** [CH03, DB68, Oni12, SSK03, YMI+21]. **input** [Hog21]. **Insertion** [HSS+04, KTA03]. **Insight** [GTB23, LSZ+99b]. **insights** [LCC22]. **Instabilities** [Cal85]. **Instability** [BE04]. **Integral** [CB92, GM91, Yan90]. **Integrals** [AYÖ17, Ave13, AA15, AA18, BL18, Gil94, HPB17, ÖÖ13, Ste73, Yas17, YÖ13, ZP17, ALA21, ALA23, KÖO23, Rui23]. **Integration** [Nal00]. **Intelligence** [Duc97, SSCL97, MP22]. **Intensities** [APNM03, BKC68, YTC+05]. **Intensity** [BWK97, MTA00]. **Intensivity** [DDPC95]. **Interacting** [KT98, MHWvdA97]. **Interaction** [ATL+18, AJ04, AA03, BMP03, Bun18, DKV+19, EGCL91, EEL96, EM17, GC92, HK03, KMJ97, KK85, KN01, LHL18, MCC03, PKYM01, Per90, PGN04, RMN+14, RFG+98, RMMP17, RP18, RT18, SBCT04a, SBCT04b,

Sab07, SS99, AA19, Bel19, CAG+21, FB20, SB07, SHBC19, SKS+19, WLM23]. **Interactions** [BP82, Bor03, CT82, DSW04, GP14, GM05, Jan65, Jeh65, KSG08, KH03, PP68, Rei73, Sau05a, FSP23]. **Interatomic** [Gon98]. **Interelectron** [AA18]. **Interest** [EBR92, MLR+98]. **interesting** [SBA+03]. **interface** [SYIY03]. **interfaces** [Per20]. **Interferences** [SS04]. **Intermediate** [LEK01, Bel22]. **Intermediates** [GAI08]. **Intermolecular** [MCG+08, MS67, Sal11, ST78]. **International** [Moh08]. **internationalization** [Kar02]. **Interparticle** [BFHS23]. **Interpenetrating** [Sil14]. **Interplay** [LDP+04, MCC03, Nal06, Sig05]. **Interpretation** [Brä04, Kar08, KP77, ST78, Ort22, NBS12]. **interpretations** [LT21]. **Interpreting** [Köv03]. **Intersection** [Pet98]. **Interstellar** [CG80]. **interstitial** [GWW19]. **Intra** [Chi03, PWZ+08]. **Intra-Hydrate** [PWZ+08]. **Intra-Site** [Chi03]. **Intramolecular** [LK14, MCG+08]. **Intrinsic** [ITI+00]. **Introduced** [KB98]. **Introducing** [Yas17]. **Introduction** [Ano19n, Ano19o, Ano19p, Sme92, TAU17, Tri90]. **Introductory** [Die97]. **Invariance** [Woo98]. **Invariances** [Kar08]. **Inversion** [GDL14, MMM18]. **investigate** [Hog21]. **Investigating** [KV08]. **Investigation** [Fuk08b, LK14, ST17, ZZ08, KÖO23]. **invoke** [Hes22]. **Involving** [Byl98, DSW04, HPB17, IL98, ALA21, ALA23, MKK+01]. **Iodine** [Mar08b]. **Ion** [Bel09, BMM13, FRM70, FAS+98, HBE+98, JJ20, Jan65, KMHL13, LJ17, Mam19, MF04, MM13, Pau13, SS04, ST07, YKC+08, Bel21, Bel22, CBSM20, MG22, SM23, VG22]. **Ion-Atom** [Bel09, BMM13, FAS+98, Bel22]. **Ion-Matter** [MM13]. **Ion-Metal** [MF04]. **Ion-Solid** [FAS+98]. **Ionic** [GL90, HPU+17, MLR+98, Sch94, FTG22]. **ionicity** [BFHS23]. **Ionization** [Bel09, BMM13, BRL13, CHR13, DC99, GS04b, GPEB21, HUS+11, HPU+17, HMH+18, MCM14, UYT97, VTM98, MG22, MU03, SM22, BG73]. **ionizations** [CCM+19]. **ionized** [MK23]. **Ionizing** [BGG+07, Fra13]. **IONO** [Mar08b]. **Ions** [Ano08h, Ano08j, ABGM03, AL04, Bic13, BKB+19, CHR13, CLK15, DGKCT15, DTC04, GP04, Khe19, LT98, MKH+97, MA04, NM03, PGJ07, RGFC13, SBCT04a, SBCT04b, SOS15, SW98, SGK+08, VI01, WMM+98, CTC22]. **IR** [CÅ01, Jan97]. **Iron** [Kot68, MKH+97]. **Irregular** [AYÖ17, SR73]. **Isaac** [Ano03a]. **ISM** [JMWG19]. **Isoelectronic** [Jør78, VI01, VT24]. **Isolobal** [YMI+21]. **Isomer** [FCC04]. **Isomerism** [Sla81]. **Isomers** [PM16]. **isospin** [YMI+21]. **Isotope** [DY08, JGNJ08, Lyo08, Mar08a]. **Isotopes** [Per98b]. **Isotopic** [BB14]. **Isovalent** [MVL01]. **Iterative** [BS05a, GDL14, SGB16]. **IV** [VT24].

J [BB21, CPBS05, DE05]. **J-coupled** [BB21]. **Jack** [OB22a]. **Jacobi** [CMDN89, CAP19]. **Jahn** [ABGM03, ADA03, BP82, BO86, Ber03, Chi03, CKRT03, DST+03, FIK+03, GWM+03, HBKS03, KH03, KBS03, LPDB03, LC03, LM03, MS03, MCC03, NeMM03, OM03, Pol03, SKT+03, SS03, SIY+19, SCN03, YAJHR03]. **Jan** [Öhr05, SBLJ05]. **Jean** [Ano19b]. **Jens** [OS05, SO05b]. **Jones** [Hal91]. **Jordan** [Brä04]. **Jørgensen** [Odd05, SBLJ05]. **Journey** [CCC17, Cra99].

Junctions [BR05].

K-edge [CCM+19]. **Kelvin** [MYM08]. **Kepler** [CCA13]. **kernels** [ORL23]. **Ket** [IM80]. **Ket-Vectors** [IM80]. **keV** [TBM01]. **Key** [RNL14, vL03, RZTSW23]. **KH** [TMK21]. **Kind** [PS05b]. **Kinetic** [CTCS05, LASV18, NA04, Per98a, YZDM01]. **Kinetic-Energy** [YZDM01]. **Kinetics** [RNL14]. **KLi** [MMSK16]. **Knowledge** [KS97b, MRS+99]. **Knowledge-Based** [KS97b]. **Kohn** [GV09, KB98, LK90]. **Kołos** [MG23a, PMK23]. **Kondo** [FCAG19, FTG22]. **Koopmans** [Ort22]. **Kossel** [Jør78]. **Kr** [PJH05]. **Kramers** [AA03]. **KS** [SKGŚ23]. **KS-DFT** [SKGŚ23]. **Kummer** [BC09].

L [OTA97, YNNU03]. **Laboratory** [KNM+08, PEMC23]. **ladder** [CAP19]. **Laguerre** [DGA18, LPC24]. **Lamé** [MFLK15]. **LaMnO** [NP03]. **Lanczos** [SP99, SGB16]. **Landscapes** [Oli12]. **Large** [Chr72, EG99, SIY+15, TTLB04]. **Large-Scale** [SIY+15]. **Laser** [AAM04, ALND10, ADA03, BS98, DGKCT15, Glu19, ML18, PR98, Per98b, TS10, VTM98, IOA03, WLM23]. **laser-driven** [WLM23]. **Laser-Induced** [TS10]. **Laser-Modified** [DGKCT15]. **Lasers** [Sva98]. **Lattice** [DDPC95]. **Lattices** [Phi98]. **Laves** [TMM03]. **law** [MG22]. **layered** [KTA03]. **LCAO** [Del74, PTC+13]. **LDA** [ABB90]. **Lead** [LvWH+01]. **Leader** [Lin99]. **Learning** [Ber02, SS17, Dra20, MP22]. **Least** [LJK+08, Löw92a]. **Least-Squares** [LJK+08]. **Legacy** [Bun17]. **Length** [PR98]. **Lennard** [Hal91]. **Lennard-Jones** [Hal91]. **Level** [MYM08, MBO+07, SPD09, SGM+13]. **Levels** [ATL+18, LJK+08, Bun23]. **Li** [BB14, Khe19, KNI+08, KNM+08, RF13, TM13, YKC+08, ŻM23]. **Li-Ion** [YKC+08]. **Li-K** [KNM+08]. **Li-like** [Khe19]. **LiAlH** [DA14]. **LiCaAlF** [ADA03]. **Lie** [AČP88]. **Life** [PB20c, BP20, SB02]. **Lifetimes** [BS98, MAS03]. **Lifting** [FSP23]. **Ligand** [ARS17]. **Ligands** [YFK+97]. **Light** [DY08, Phi98, SBH+20]. **LiH** [PS05a]. **Like** [FPL97, RLF17, BH24, CKC09, Khe19, Lau09, VT24]. **Limit** [Bas78, Sau05a]. **Limited** [LK09]. **Limits** [Brä12, Ber02]. **Linderberg** [Öhr05, SBLJ05]. **Lindgren** [Löw98, Nor98]. **Line** [Eks98, HBKS03]. **Linear** [AL04, BR82, Bas78, BB13, Bis94, JJD05, Kla81, LGJP99, LPDB03, LDNP99, Löw92a, Löw96b, MCA+18, PS05a, PM16, Tap09, BLC23, PS05b]. **Linear-Response** [MCA+18, PM16]. **Linearized** [SED+98]. **Linearized-Augmented-Plane-Wave** [SED+98]. **Lines** [Glu19]. **Linked** [Bra77]. **Linked-Cluster** [Bra77]. **Liouvillian** [Löw85c]. **Liquid** [BRL13, Krs16, MLR+98, RFG+98, YKY+00]. **Liquids** [HPRR10]. **LiRb** [SM23]. **List** [Ano64d, Ano65d, Ano67e, Ano68e, Ano70e, Ano72e, Ano73e, Ano74c, Ano75c, Ano77d, Ano78c, Ano80e, Ano81i, Ano81j, Ano04i]. **Lithium** [YKC+08, KTA03, LYM03]. **Lived** [Lyo08, SM22]. **living** [Per20]. **LiX** [BJMB14]. **Local** [GL90, JcH18, Köv08, LLBK+98, MMM18, Nes03, PWZ+08, YIYM03].

Local-Scaling [LLBK+98]. **Localizability** [ACDK72]. **Localization** [GM17, PLA01]. **Localized** [CE78, KT98, KTC01, Nal09, MG21]. **Locally** [SPAS05]. **Loge** [ACDK72]. **Logical** [Brä12]. **lone** [AR03]. **Long** [DB13, JGCRC16, Lyo08, SM22, TMMS10]. **Long-Lived** [Lyo08, SM22]. **Long-Range** [DB13, JGCRC16]. **Loss** [AJ04, AL04, Bel09, Bic13, GS04b, Kho04, Tők19]. **Loss-Excitation** [Bel09]. **Loss-Ionization** [Bel09]. **Lost** [Heh18]. **Low** [DLMS03, DST+03, Jos08, KM98, LP97, LKD05, MF04, MMSK16, Nes75, RPSB00, SPD09, Sim07, SSS05, TM13, Bel19, Kar24]. **Low-dimensional** [SPD09]. **Low-Energy** [Sim07, SSS05]. **Low-Lying** [KM98, LKD05, MMSK16, TM13, RPSB00, Bel19]. **Low-Spin** [LP97]. **Low-Temperature** [DLMS03]. **Löwdin** [Bun17, Heh18, Kar02, LÖS02, LÖBS17, SB02, SB17a, SPH14]. **Löwdin's** [SS17]. **Lower** [BB14, Wei72]. **lowering** [TSTH03]. **Lowest** [GV09]. **Lunell** [Miy03]. **Lying** [KM98, LKD05, MMSK16, TM13, Bel19, RPSB00].

M&S [TR14]. **machine** [Dra20]. **Macrocyclic** [YFK+97, ZDZO11]. **Made** [Col68]. **Madelung** [KSY08]. **Magic** [KMR01]. **Magnesium** [MYM08]. **Magnesium-Zinc** [MYM08]. **Magnetic** [Bel06, BB11, CE72, DST+03, DeB09, GWM+03, IS01, JH99, JcH18, Laz04, Ram08, VRG90, Vis05, BB22a, TMM03]. **Main** [Dau64]. **make** [KHPP23]. **Making** [MKH+97]. **Maleonitrile** [RGA99]. **Manganese** [NeMM03]. **Manifestations** [SBC+03]. **Manipulation** [MCP12, WMM+98]. **Many** [AO03, AA01, Ave98, BŚG14, CB92, Cru09c, DDPC95, DSR81, HG17, HW01, HMW01, IOA03, Khe19, KT98, KB86, Löw88b, LFM89, MC10, Mat78, Mic15, Mic17, MK18, Nic17, NM03, PKYM01, RP72, Sal74, SW98, WDD16, vL03, LSZT90, Mic02, Mic22]. **Many-Atom** [HG17, Mic15, Mic17, Mic02, Mic22]. **Many-Body** [AA01, BŚG14, DDPC95, HW01, HMW01, Khe19, KT98, KB86, MC10, Mat78, MK18, SW98, WDD16, vL03]. **Many-Electron** [Ave98, DSR81, Nic17, PKYM01, RP72, Sal74, AO03, Cru09c, IOA03]. **many-fermion** [LSZT90]. **Many-Particle** [Löw88b, LFM89]. **Maruani** [Ano19b]. **Mass** [KS88, Lyo08, Mar08a, MRS+99]. **Mass-Independent** [Lyo08, Mar08a]. **Masses** [SBF+08]. **Master** [Kai15]. **match** [SÁ23a]. **Material** [FE97, GP14]. **materialism** [PB20a]. **Materials** [Ber14, DLMS03, Kuk14, MF14, Oni12, Oni15, SNIM08, TR14, AO03, LSZ+00, SBA+03, Sab14a]. **Mathematical** [CD05, EBR92, Gut06, Sut01, SCT15, SCT16]. **Matrices** [BMP03, BK70, Dah01, Har90, Kry81, RP72]. **Matrix** [LK90, McW98, Mic99, PKYM01, RPSB00, RP72, Öhr02]. **Matter** [Ano19j, Ber03, DTC04, Gre08, MM13, SBCT04a, SBCT04b, AA19]. **MCSTEP** [Yea05]. **Mean** [CTC22, HG17, SOS13, SOS11, SOS15, CTSSO19, CTO22, SSO19]. **Mean-Field** [HG17]. **meaningful** [SKGŚ23]. **Means** [ST78]. **Measured** [BS98, NHYU03]. **Measurements**

[BLKS78, KNM+08, MRS+99, MYW00, Tap11]. **Mechanical** [And80, AA01, Bel09, BB17, CC97, HPRR10, KZR86, Pul77, Wei72, vS07, BMR+24, NBA20]. **Mechanics** [Brä08, CCM05, CL05, Deu99, MDÖ05, Öhr17, PD10, Sch94, Sig05, Spe78, TL10, CCT02, LT21, MG21, SBC10]. **mechanics/extremely** [MG21]. **Mechanism** [Ber03, Oni15, TBM01]. **Mechanisms** [ASGG08, FHHZ88, YAJHR03]. **Mechanistic** [BB13, BB15, Mar08a]. **Media** [AGMdV+13, JJD05, Kar97]. **Mediated** [MBM99]. **medical** [BB21]. **membered** [BMC97]. **Memory** [SS17, JJ20, MG20]. **Mercury** [ASGG08]. **MEST** [Hog13g, Hog14]. **Metal** [Ada97a, ARS99, BU97, EGCL91, GP14, Kap98, KMR01, MF04, RR05, SS98, SNM+97, SNIM08, SCN03, TLOK97, Tak19, TTLB04, FB20, FCAG19, FTG22, Hog23c, KBH23, MGAUP23, PBOL02, STO+00, SYIY03]. **Metal-Cluster** [KMR01]. **metal-film** [KBH23]. **Metallic** [Bro98a, Bro98b, Saa01, AMAA22]. **Metalloporphyrins** [DRV82]. **Metals** [Ber74, FHHE82, MA04, SED+98, STO+00]. **Metastability** [PB14]. **Metastable** [CKRT03]. **Methane** [RZTSW23, Hog23c, HDFT24]. **Methanol** [FCC04]. **Method** [Ada97b, Ada00, Ave98, CTCS05, CL00, CB18, DKMP98, EG99, FSB+97, FCH15, Fuk15, GW17, GEO91, GVFR98, Glu19, GDL14, I'H64, IFAY08, KE97, LEK01, Löw88b, LFM89, Löw92a, LM92, MW08, May80, MMM18, MM96, Mon05, MKK+00, Mur08, MKB04, MMSK16, Nak00, NFW+98, OW08, OE17, PB99, RPSB00, RP18, SGB16, SS99, SNMI00, Sla64, SGM+13, TMN10, TAM04, WD70, WmG18, Yea05, BH24, DAB+23, GPEB21, Hog23c, HDFT24, KBH23, LMK19, MKK+01, ÖEO23, TMK21]. **Methodologies** [BRL13]. **Methodology** [GDL98, ZLC+10, CCT02]. **Methods** [AdMB99, AČP88, AH19b, And80, ACDK72, Bel09, Byl98, Dau64, FP06, GC92, HPU+17, Har04, Hät05, HZ89, HG17, HM21, HMW01, JG08, LGJP99, LJKH13, LB92, Löw85c, ML18, Mic74, Mic17, MP89, Nic10, ÖÖ13, PS05a, RR05, STZY18, San98, Sau05b, SBK15, TAU17, TL10, WN05, WDD16, Bar23, CCM+19, EÜSB21, Hog14, JMWG19, LH20, Min22, SBGJ08, SBC10]. **Methylamine** [SSV98]. **Metrology** [PR98]. **MeV** [AGO07, WHB+24]. **Mg** [FU00, NHYU03]. **Mg-** [NHYU03]. **MgB** [SCE19]. **mGluR5** [ST17]. **MgO** [OTA97]. **MI** [GVFR98]. **Michael** [Sab00]. **Microscopic** [Chi03, MTS04, Brä02]. **Minimum** [Kou15]. **Mixed** [MLR+98, Mon05, PSAP10, SIY+19]. **Mixed-Quantum** [PSAP10]. **Mixed-Quantum/Classical** [PSAP10]. **Mixed-Valence** [SIY+19]. **Mixing** [AR03, SH95]. **mixture** [LCC22]. **MM** [BBB10, MC10, SBC10, SIY+15, TL10, ZLC+10]. **Mn** [NeMM03, YNNU03]. **MnO** [GWM+03]. **MO** [Yas17, CDP82, Del74, YNNU03, RZTSW23]. **Mo-** [RZTSW23]. **Mobile** [KTMA08]. **mobility** [ZLL+20]. **Model** [ABC+98, BMPV99, BGW73, BB13, BE04, BG73, BWH08, BC09, Cam12, Dru78, DB01, Gre73, GM05, GVFG09, HS86, HSR98, JGCRC16, Jos08, Kap98, Kri03, KMR01, LS07, MS03, PJH05, Sme99, VG22, DAB+23, NA19]. **Modeling**

[DNM+14, GVFG09, Köv08, Kuk14, MHWvdA97, RMN+14, TL10, HDFT24]. **Models** [Ano04l, BB15, BRL13, GV09, KGW98, KE00, MBO+07, NA04, Nik70, SIY+15, AA19, MK23, SS22]. **Modern** [CTG98, HPL98, KK85, SL20]. **Modified** [DGKCT15, KN01, BGW73]. **Modulators** [ST17]. **Module** [PM16]. **MoF** [MKK+01]. **Molecular** [ÅCL92, Ada97b, ADRAB16, AH19b, AGL05, ALND10, Ave13, AA15, BGG+07, BVHK03, BLC23, BU97, BHV+00, Bas64, Ber03, BWK97, BR05, Bis67, BC80, Brä19, BJV86, CTSO04, CCVB94, CMJR+04, Cio90, CCA13, CS04, CLK15, DB68, Dau64, DNM+14, Dru78, DW98, Fra13, FF72, GP91, GM17, Gil94, GL90, GM91, Hal64, Hal91, HS19, Har67, HZ89, HJ88, HPRR10, Hog13g, HBGvM19, IFAY08, ILS08, Jan97, Jeh65, JH99, JS21, JcH18, KS77, KS88, KSG08, KD11, KTC01, Kry03, Löw80b, LÅJM95, MW08, Mic74, MT04, MWL+05, MKK+00, MP97, MBO+07, Nal09, NM03, ODE75, Ohn67, ÖB81, Öhr15, Oli12, OK11, OBHM17, PTC+13, PWZ+08, Pul77, QGW01, RMN+14, RFG+98, Ray95, Rei73, RM04, Ryc98, SBH+20, Sal11, San98, San92, Sch94, ST78, Sim99, Sjö04]. **Molecular** [Ste73, ST07, Sut97, TAM04, TL10, TM21, Uda00, VWP+98, Yan81, Yas17, dLHD10, Bis19, BSL+19, CAP19, KÖO23, LSC19, MG21, Nal23, NBA20, ÖEO23, PEMC23, RSP21, SBLJ05, SBC10, SM22, SM23, SA23b, Yas23, ŻMM23]. **Molecular-Dynamics** [BHV+00]. **Molecular-Orbital** [MW08, JS21]. **Molecule** [Apo01, Bro98a, Bro98b, CT82, FRM70, FPL97, GM05, JSG+14, Kom05, KMJ97, LKD05, Löw65c, MW98, MCM14, MSM17, OM03, STZY18, Sim05, LMK19, PMK23, SZP21, WLM23]. **Molecule-Ion** [FRM70]. **Molecule-Particle** [GM05]. **Molecules** [ÅVM96, AAE+01, AAM04, ACDK72, BND81, BJMB14, BO86, CE72, Cam12, CL05, CG80, CKC09, Chr72, CLÅ05, Dau70, Del74, EG99, ERC88, FLV99, FVB99, FMA08, GSTvE98, GCAGM17, GNM08, HL97, IBB+19, IS01, Jan97, Kar97, KGW98, KMHL13, Kob97, LR72, LASV18, Lyo08, ML18, Mat96, MFLK11, MKN10, MK18, MTA97, Nal06, Nes67, Nic10, OO05, OBHM17, PB14, PGP17, PBK04, Rei73, RGFC13, RP18, Ser74, Sme92, SSV98, SCTH+07, Sut01, UK05, YTF78, YTC+05, ZDZO11, BLC23, CM24, HO16, MKK+01, QSW20, YMI+21]. **Møller** [GC92, OB23, VI01, GS04a]. **Møller-Plesset** [GS04a]. **Molten** [MKH+97]. **Moment** [RM04, SJO05, YÖ13, PS21]. **Moments** [AB73, BO86, BWK97, Eks98, Glu19, PJH05, Woo98]. **Momentum** [BLKS78, KS77, MTS04, MFLK15, OE17, TM13, WP06, AP03]. **Monoclinic** [DA14]. **Monohydrated** [Tak19]. **Monomer** [PWZ+08]. **monovalent** [FB20]. **Monte** [SH19, AGL05, CCT02, CCM05, CC97, HB14, Hog18e, Hog21, Hog23c, HDFT24, KBH23, MCA+18, NFW+98, RMMP17, RP18, TAU17, vS07]. **Monte-Carlo** [CC97]. **Morse** [Apo01]. **Motion** [Löw85c, Per17, Sch94, Sut97, WN05, YTC+05, MKB04, NBA20]. **Mountains** [Kai15]. **MP2** [JSF08, WmG18]. **muffin** [GWW19]. **muffin-tin** [GWW19]. **Multi** [CLÅ05, MDBM98, PWZ+08, SPD09, LH20, FSP23].

multi-CPU [LH20]. **Multi-electron** [SPD09]. **Multi-Hydrates** [PWZ+08]. **Multi-Photon** [CLÅ05]. **Multi-reference** [MDBM98]. **Multicenter** [ALA21, HPB17]. **Multichannel** [Shi12]. **Multicharged** [BKB+19, Khe19]. **Multiconfiguration** [PGP17, WD70]. **Multiconfigurational** [LJKH13, STZY18, Yea05]. **Multidimensional** [Pol03]. **Multielectron** [KGI+19, OW08]. **Multiphonon** [HK03]. **Multiphoton** [Glu19, VTM98]. **Multiple** [Nal09, SBDD03, ST07]. **Multiplet** [IOI+00, ITI+00, OYI+00]. **Multiply** [AK12, CHR13]. **Multipole** [BO86, Woo98, YÖ13]. **Multireference** [BB99b, EM17, HMW01, LGJP99, LF09, MH98, MSM17, VI01, JMWG19, LH20]. **Multireference-Coupled** [MSM17]. **Multireference-Fock** [BB99b]. **Multiresolution** [DGKCT15, Bis19]. **Multiscale** [TR14]. **Muonium** [Hug98]. **Mutations** [Löw65c]. **myelinated** [JJ20].

N [JMWG19, BMC97, HSR98, Mur03, TBM01]. **N'-Tetramethyldiamide** [HSR98]. **NaEuCl** [APNM03]. **NaH** [LMK19]. **NaK** [MSM17]. **nano** [SBA+03]. **Nanoclusters** [ARS17]. **Nanodosimetry** [Bic04]. **Nanometer** [Ros98]. **Nanoparticles** [GP14, OBHM17, AMAA22]. **Nanoplasmas** [LJ17]. **Nanostructures** [DO09, AGS+19]. **Nanotubes** [AAM04, LYM03, MOB+03]. **nanotubes-gold** [MOB+03]. **NaSmCl** [APNM03]. **native** [YMI+21]. **Natural** [AT91, AAG03, AAAC04, BK70, Dav72, MGAUP23, MPU19]. **Nature** [Brä04, Sjö04, YM97]. **Near** [KsKsN08, MYW00, MYM08, NHYU03, YFK+97]. **Near-Edge** [KsKsN08]. **Nearly** [Lin17a]. **Necessary** [Brä04]. **Negative** [Kom05, SW98]. **Neon** [Sab97]. **Network** [PWZ+08]. **Networks** [SIY+15]. **neural** [MG20, Per20, Rou20]. **Neutral** [DNM+14]. **Neutrino** [KS88]. **neutron** [Kar24]. **Newton** [GDL14, HZ89]. **Next** [SO05a]. **NH** [Sau05b, YTC+05]. **Ni** [SMAS08, Hog23c, HDFT24, KKA97, WHB+24, YKY+00]. **Nitrate** [HBT+00]. **Nitrates** [HTS+00]. **Nitric** [BWH08]. **Nitrides** [TLOK97]. **Nitroaniline** [CCCC15]. **Nitrogen** [RNL14, VI01]. **Nitrones** [RGA99]. **Nitroprusside** [CKRT03]. **NMR** [BB17, BB21, BB22a, CPBS05, PB05, SPAS05]. **NO** [SP99]. **NOCV** [ŻMM23]. **Noise** [DeB09]. **Non** [AHPD+03, AL04, AR03, BVHK03, BS05a, Bis94, KNN17, NBA20, PS05b, Sau05a, Sim99, Sme92, BMR+24, SA23b]. **Non-Adiabatic** [BVHK03, Sim99, BMR+24]. **Non-Born** [NBA20, SA23b]. **Non-Condon** [AHPD+03]. **Non-Coulombic** [KNN17]. **Non-degenerate** [AR03]. **Non-Iterative** [BS05a]. **Non-Linear** [AL04, Bis94, PS05b]. **Non-relativistic** [Sau05a]. **Non-Rigid** [Sme92]. **Nonadditive** [Kap98]. **Nonadditivity** [MS67]. **Nonadiabatic** [Kry03, Nik70, SP99]. **Noncanonical** [LB92]. **Noncovalent** [DSW04]. **Nonempirical** [PB75]. **Nonequilibrium** [KD11, NTT20]. **noninteger** [GJP23]. **nonintegral** [Wen21]. **Nonlinear** [IBB+19, LHL18, MFCT15, MA04, OO82, PGN04, RAR15, BLC23, LCC22].

Nonlocal [LV90, Nes03, Sjö04]. **nonorthogonal** [SKS+19]. **Nonorthogonality** [Löw70b]. **Nonparametrized** [HPRR10]. **Nonrelativistic** [Öhr16, SA23b]. **nonrepresentational** [LT21]. **Nonrigid** [Ser74, SSV98]. **Nonstationary** [Nic17]. **Normality** [IM80]. **Normalizing** [GWW19]. **Notes** [Ano99a]. **Novel** [IFAY08, Mat96, Oli12, LT21]. **Nuclear** [CTSDÖ04b, JcH18, LDB95, Lon99, PSAP10, Ray95, Sab97, SPAS05, SGM+13, Sut97, Vis05]. **Nuclearity** [Bor03]. **Nucleation** [NAY+08]. **Nuclei** [BRL13, DY08, Eks98, Glu19, Bel21, NBA20]. **Nucleic** [CL07, PP68, Tur07]. **nucleosome** [FB20]. **Nucleotide** [ZDZO11]. **nucleus** [LSC19]. **Number** [Ono00, TM13]. **Numbers** [ATL+18, KMR01]. **Numerical** [BS05a, Gut97, Kou15, Lin17b, MK18, Sid18, BG23].

O [CL00, OTA97, SIY+19, YKS+12, ŻM23, CSZ99, BMC97, BRW08, MKK+00, Sau05b]. **o-C** [CSZ99]. **Obituary** [Ano03h, Sab00]. **Objects** [EBR92]. **Observation** [Tos08]. **Observed** [Miy03, SEL01]. **Obtained** [MMM18]. **Obtaining** [HZ89]. **Occupancy** [SBDD03]. **Occurrence** [Löw88b, LFM89]. **Oddershede** [OS05, SO05b]. **OEC** [YKS+12]. **OEP** [BŚG14]. **Off** [DB13]. **Off-Diagonal** [DB13]. **oganesson** [GPEB21]. **OH** [GAI08, PEMC23, RRMAF08]. **Öhrn** [Lin99, LSZ+99b]. **OKa** [MKK+00]. **Oligomers** [CÅ01, PM16]. **Olov** [Bun17, Heh18, Kar02, LÖS02, LÖBS17, SB02]. **On-Line** [Eks98]. **One** [AYÖ17, ARS99, Bel21, BC80, FP06, FCH15, GW18, Kar24, LK13, MM96, OM03, Ort99, SBC09a, SPM09, SAL10, SGK+08, GVFR98]. **One-** [BC80, FP06, LK13, OM03, SGK+08]. **One-Dimensionally** [FCH15]. **One-Electron** [AYÖ17, Ort99, SPM09]. **One-Particle** [GW18]. **One-Photon** [SAL10]. **Ones** [Lin17b]. **Only** [PTC+13]. **Open** [Bad09, Bra77, CG80, Cru09c, FMA08, GC10, GVFR98, LP97, MP89, RTV05, YMI+21]. **Open-Shell** [Bra77, FMA08, GVFR98, LP97, MP89, RTV05, YMI+21]. **Operator** [LMSP01, Löw67c, MT04, Pal04]. **Operators** [FP06, HMC73, Löw96b, MKB04, SS03]. **Oppenheimer** [TA04, NBA20, SZP21, SA23b, Tap01]. **opposite** [SS22]. **Optical** [BMPV99, Bis94, DO09, DA14, HDB03, KsKsN08, MCP12, ML18, PR05, Phi98, RDNFH98, IOA03]. **Optimization** [BHM17, CMDN89, CTG98, HZ89]. **Optimizations** [Hät05]. **Optimized** [GW01, Khe19, KKGG98, WD70, SKGŚ23]. **Orbit** [ÅVM96, ERC88, LF09, RM04]. **Orbital** [Ada97b, AT91, ADRAB16, CTCS05, Cio90, DB68, FF72, GWM+03, Hal91, Har67, IFAY08, KT15, MW08, MNR+98, MKK+00, Nal09, NSM11, ODE75, Ohn67, San92, TSON00, UYT97, Uda00, Yas17, CTSSO19, CTO22, CTC22, JS21, MG21, MGAUP23, MPU19, PEMC23, SCJ+23, Yas23]. **Orbital-Communication** [NSM11]. **Orbital-Free** [KT15]. **Orbital/Plane** [Mon05]. **Orbitals** [AYÖ17, AAG03, AAAC04, AA15, BŚG14, CE78, CB92, CCA13, Dav72, DR90, GM17, Hog13g, HPB17, HM21, KTC01, Lin17b,

PTC$^+$13, PTBH13, RP72, Ste73, Yan81, CAP19, KÖO23, LSC19, Rui23]. **Order** [AAM04, BS05a, BB99b, DB13, Hät05, IL98, KB86, KNN17, LDB95, MW98, RR05, SW98, SPH14, VTM98, AHPD$^+$03, Bar23, GJP23, MCC03, VdLCPT98]. **Ordered** [DLMS03]. **Ordering** [CCVB94, GWM$^+$03]. **orders** [Wen21]. **Organic** [BMPV99, Dau70, GAI08, Sey12, GTB23, YMI$^+$21]. **Orientational** [CTSDÖ05]. **Origin** [CKRT03, FRM70, OM03, RGA99]. **Ortho** [DNM$^+$14]. **Ortho-Anisidine** [DNM$^+$14]. **Orthogonal** [DGA18, CAP19]. **Orthogonality** [IM80]. **Orthogonalization** [Sri01]. **Orthogonalizations** [SS17]. **Orthonormal** [CCA13, RP72]. **oscillating** [ALA23]. **Oscillation** [BS72]. **oscillations** [JJ20]. **Oscillator** [BLKS78, CTSOS99, CTSO04, Khe19, KMR01, OOSS17, CTSSO19]. **Oscillator-Strength** [OOSS17]. **Osvaldo** [Ano04i, SBK04]. **Other** [ASGG08, BGG$^+$07, ERC88, Löw92a, Ram08, SBA$^+$03]. **Overlap** [FH65, ÖÖ13]. **Overview** [vS07]. **Oxidation** [SIY$^+$15, ZZ08, YMI$^+$21]. **Oxidation-Theoretical** [SIY$^+$15]. **Oxide** [GP14, SNIM08, YKC$^+$08, CCL03, Fuk03, Sak03b]. **Oxides** [EGCL91, KIT$^+$08, PBOL02]. **Oxonium** [LM97]. **oxy** [RZTSW23, YMI$^+$21]. **oxy-radicals** [YMI$^+$21]. **Oxyanions** [Cse97]. **Oxygen** [Mar08a, MKH$^+$97, NM00, SIY$^+$15, SIY$^+$19, MFMCN01, Sak03a, YMI$^+$21]. **Oxygen-Evolving** [SIY$^+$15]. **Oxygenated** [GAI08]. **oxygenation** [YMI$^+$21]. **Oxynitride** [KsKsN08].

P [CSZ99, Bel19, OM03]. **Packages** [LBH$^+$17]. **Packets** [SAL10]. **Padé** [Bel06, BB13, DeB09]. **Page** [Ano09d, Ano12h, Ano14e, Ano15g, Ano15h, Ano16d, Ano17j, Ano17k, Ano17l, Ano18d, Ano19q, Ano19r, Ano20g, Ano20h, Ano21g, Ano21h, Ano22h, Ano22i, Ano23g, Ano23h, Ano24d, Hog18f, SB13e, Ano64c, Ano65c, Ano67d, Ano68d, Ano70d, Ano72d, Ano73d, Ano74b, Ano75b, Ano77c, Ano78b, Ano80c, Ano81e, Ano81f, Ano82f, Ano82g, Ano85d, Ano86a, Ano88c, Ano89c, Ano90b, Ano91b, Ano92c, Ano92d, Ano94c, Ano95b, Ano96b, Ano97d, Ano97e, Ano98j, Ano98k, Ano98l, Ano99f, Ano99g, Ano99h, Ano08e, Ano08f, Ano09e, Ano09f, Ano12d]. **Pair** [MS65, TM13]. **Pair-Correlated** [MS65]. **Pairs** [AR03, AA03, KN01, AP03]. **Panexperiential** [PB20a]. **Paper** [Hal91]. **Paradigms** [MDBM98]. **Paradox** [McW99]. **Parallel** [HS19, PM16, LH20]. **Parallelization** [TR98]. **Paramagnetic** [Kot68]. **Parameter** [Apo01]. **Parameterization** [AR03]. **Parameters** [GM05]. **Parametric** [Bel11]. **Parametrization** [ACDV01]. **parity** [QSW20]. **Parrinello** [PWZ$^+$08]. **Part** [SBCT04a, SBCT04b, SBC09b, SBC09a, LSZ$^+$98b, LSZ$^+$98c, NBS10, SBM$^+$01a, SBM$^+$01b, Löw88b, LFM89, NBS12, SCT16]. **Partial** [PSS98, SGB16]. **Partial-Wave** [PSS98]. **Participants** [Ano97a, Ano98t, Ano98u, Ano01m, Ano01n]. **Particle** [BGW73, BG73, BC00, CB18, GW18, GSTvE98, Gre73, GM05, IKN$^+$08, KV08, Löw88b, LFM89, SS03, Sig05, Uda00, FB20, GJP23, SA23b]. **Particles** [AJ04, BRL13, Fra13, PGN04, RDNFH98, TTLB04, AGS$^+$19, BKL21, Tők19].

Partition [Nak00]. **Partitioning** [Lar02, Löw98, Mic17]. **Parts** [ÖÖ13]. **Passage** [ML18]. **Passivation** [ARS17]. **Path** [BŚG17, GM91, LPDB03, Nag01]. **paths** [BSL+19]. **Pathway** [HS19]. **Pauli** [LASV18, SO19c]. **Pb** [KIT+08, HHU+21, LvWH+01, MLR+98]. **PbO** [RM04]. **PCM** [Cam12]. **Pd** [CMVPFC16]. **PEDICI** [TR98]. **Peierls** [BE04]. **Pendulum** [PS05b]. **Per-Olov** [Bun17, Heh18, Kar02, LÖS02, LÖBS17, SB02]. **Perchlorate** [Lin05]. **Perform** [PTC+13]. **Performance** [PM14, CCM+19]. **Periodic** [ABB90, FCH15, Gon98, LBV01, Mon05, Ros98]. **Perovskite** [GWM+03, KIT+08, SKT+08]. **Perovskite-Type** [SKT+08]. **Perspectives** [Bel11, CL05, Del74, Nal03, OPPZ06, PTLGOM12, SBG+98, Brä03, SBM+01a, SBM+01b]. **Perturbation** [Bra77, FMA08, GC92, Gon98, GS04a, GS04b, HBE64, HW01, Khe19, KMJ97, KB86, Lau09, LP97, Lin17c, PČ75, RR05, SW98, VI01, KHPP23, LH20, OB23]. **Perturbative** [BE01, BB99b, Bar23]. **PESA** [NHYU03]. **PET** [BWVD+13]. **Pharmacology** [Pul77]. **Phase** [Dah01, DLMS03, GSWW10, HSR98, MRS+99, MCC03, RAR+08, TMN10, TMM03, TSTH03, Yam03, YIYM03]. **Phase-Space** [Dah01]. **Phases** [DA14]. **Phenomena** [ÅVM96, Löw67c, Sri01]. **Phenomenological** [Kar08]. **Phenyloxirane** [JJD05]. **Phonon** [HBKS03, MS03, SHBC19]. **Phonon-assisted** [MS03]. **Phosphorus** [OM03]. **Photobiological** [GBPSR10]. **Photochemical** [Dau70]. **Photodetachment** [HHK+98]. **Photodissociation** [JGNJ08]. **Photodissociations** [LF09]. **Photodynamic** [MM99]. **photoelectrochemical** [PBOL02]. **Photoelectron** [Ada97b, BB99b, Jør74, Jør78, Köv08]. **Photoexcited** [Mic15]. **Photoionization** [Dol09, GCAGM17, MTA00]. **Photolysis** [KLG+08, Lyo08, BTB+20]. **Photon** [CLÅ05, SAL10]. **Photonic** [Tap17]. **Photophysics** [FLV99]. **photosynthesis** [YMI+21]. **Photosystem** [SIY+15, SIY+19]. **Physical** [BS04, Brä12, GM05, LB92, Rei73, SSCL97, BFHS23, PB20a]. **Physically** [SKGŚ23]. **Physicochemical** [TY85]. **Physics** [BVHK03, Bel11, BR20, Cal13, CT82, Dru78, EBR92, Jan65, Nor98, PD10, PR98, SBF+08, SBK15, Sut97, Sut98, Brä03, HPL98, LSZ+98b, LSZ+98c, SBM+01a, SBM+01b, SBC+03, SBSL08, SCT15, SCT16]. **Physisorption** [SH19]. **Pi** [BS72, Lyk64]. **Pi-Electron** [BS72, Lyk64]. **Picture** [GSTvE98, Ort99, ŻMM23]. **Pictures** [Sim99]. **Pionic** [DKV+19]. **planar** [YFK+97]. **Plane** [SED+98, Sla64]. **Plane-Wave** [Mon05]. **Plasma** [SCM09]. **Plasmas** [BKB+19]. **Plasmon** [AGS+19, JJ20, VG22]. **Plasmonic** [ARS17]. **plasticity** [Sak03b]. **Platinum** [HB14, Hog21]. **platinum-doped** [Hog21]. **Plesset** [GS04a, GC92, OB23, VI01]. **Podolsky** [McW99]. **Point** [CCC17, ST17]. **Poisson** [BS05a]. **Polarizabilities** [AB73, AAAC04, BO86, CMFA99, PM16]. **Polarizability** [CCM05, Kom05, PS05a, RM04, PS21]. **Polarizable** [ABC+98, Cam12, JGCRC16, LJKH13, OK11]. **Polarization**

[CTCS05, GEO91, Odd78]. **Polish** [MG23a]. **Polyacetylene** [BE04, För94]. **Polyatomic** [AK12, Rei73]. **Polycrystalline** [HSS+04]. **Polyelectronic** [MKN10]. **Polyenes** [Bas78]. **Polymerization** [MW08]. **Polymers** [And80, CMFA99, DDPC95, DC99, Ker82, LBV01, RPSB00, SD04]. **Polynomial** [Yas17]. **Polynomials** [DGA18, CAP19]. **Polypeptides** [dLHD10]. **Polypyridine** [CÅ01]. **Populating** [Coo18]. **position** [ÖEO23]. **Positron** [BWVD+13, FJS+04, AP03, MAS03, SSK03]. **Positron-Electron** [FJS+04]. **Positron-Emitters** [BWVD+13]. **Positronic** [Shi12]. **Positronium** [Hug98]. **positrons** [AA19, SJAB+22]. **Possible** [Moh08]. **Post** [TA04]. **Post-Born** [TA04]. **Potential** [Apo01, BB99b, Dru78, GMLSC+10, GW18, HBT+00, KSY08, KB98, KKGG98, LBH+17, LRCR98, LMK19, MFCT15, MCM14, MMSK16, MSM17, Nag01, Nes98, Nes03, PTBH13, RFG+98, SJO05, SED+98, Sil14, SM23, ŻM23, LPC24, SKGŚ23, TMK21, ŻMM23]. **potential-based** [ŻMM23]. **Potentials** [Kap98, MMM18, ST78, ŚBG14, GPEB21, KTA03, MMM19, SZP21, SO19c]. **Poul** [Odd05, SBLJ05]. **Power** [McG04, NA04, Pau13, Por04, SO05a, SRZE04, Sva98, Wei04, BG23, MMM22]. **Powers** [AGO07, CTSO04, PGJ07]. **Practical** [GVCN82]. **Precise** [SBF+08]. **Precision** [LJK+08, Hug98, RSP21, San98]. **predicted** [Mur03]. **Prediction** [FU00, IFAY08, KZR86, Tos08, Ort22]. **Predictions** [CO17]. **Predissociative** [Lyo08]. **Preface** [AUS00, AUW03, AH19a, Ano99o, Ano01l, Ano03i, Ano03j, Ano04j, Ano04k, Ano08k, Ano11h, Ano11i, Ano12g, Ano13i, Ano22g, BG01a, BG01b, BS05b, BS06, BS07, Brä21b, BB24b, CTS15, CTS16, Can10, Cru09a, Cru09b, HP98, Hog13f, HO17, Hog18a, Hog23b, JKMB19b, KS97a, Kle08, KOS99, LB99, Löw64b, Löw65b, Löw67b, Löw68b, Löw70c, Löw72b, Löw73b, Löw74b, Löw75b, Löw77b, Löw78b, Löw80c, Löw81c, Löw81d, Löw82c, Löw82d, Löw85b, Löw86b, Löw88c, Löw89, Löw91, Löw92b, Löw92c, Löw94, Löw95, Löw96a, MH21, MG23b, NB10, OB22b, OJ05, PB20b, RB20, SB09b, SB12b, SB13d, Sab14b, SB15, SB17c, SB17d, SB18b, SO19a, Sem98, Wil98a, Wil98b]. **Preliminary** [Gos02a, KGW98]. **Present** [Bun18]. **Preserving** [Lev14]. **Pressure** [GVFG09, MF14, ST17, Yam03]. **pressure-induced** [Yam03]. **Prevention** [MCP12]. **Previous** [Ano67b, Ano68b, Ano70b, Ano72b, Ano73b, Ano74a, Ano75a, Ano77a, Ano78a, Ano80a, Ano81a, Ano81b, Ano82a, Ano82b, Ano85a]. **Primitive** [SW98]. **Primitives** [KGW98]. **Principal** [Öhr17, Tew21]. **Principle** [HPRR10, LFM89, WT99]. **Principles** [Ada97b, Brä12, CCVB94, DA14, Fuk08a, Fuk08b, HBGvM19, IOI+00, KIT+08, KSY08, MTS04, OYI+00, YKC+08, KTA03, Sak03a, Yam03]. **Probabilities** [VI01]. **Probability** [GL68]. **probe** [SM22]. **Probes** [CPBS05]. **Probing** [Nal06]. **Problem** [DSR81, DST+03, HW01, Hyl64, KS88, KO18, Löw70b, Mat78, MP89, Nic17, SB99, Sut97, vL03, BKL21, Lin02]. **Problems**

[AA01, CTCS05, Del74, GAM+13, Har04, Har05, Kar08, Ler85, LB92, Löw65c, OO82, Sut01, YTF78, Gos02b, SSK03]. **Procedure** [CMDN89, PSS98]. **Proceedings** [Hog13g, Hog14]. **Process** [UYT97, AO03, SKS+19]. **Processes** [ALND10, BGG+07, Brä04, CTSDÖ04a, GBPSR10, HL97, LA12, MCG+08, MF04, MM13, MHWvdA97, MA04, Öhr15, OO82, PSAP10, RNL14, Tap01, Tap09, BLC23, Dur20, LSZ+99a, LSZB00, MMM19]. **Processing** [BB11, BB17]. **Produced** [LS07]. **Product** [PTBH13, LPC24]. **production** [Hog21, HDFT24, KBH23]. **products** [SCJ+23]. **Professor** [SBK04]. **Profiles** [KS77, OE17, ÖEO23, VG22]. **Program** [KTC01, Lad73, TR98]. **Progress** [ADRAB16, Ort22, SBC10]. **Projected** [May80, Sme99]. **projectile** [CTO22]. **Projection** [HMC73]. **Projections** [CL05]. **prolate** [MFA21]. **Propagating** [LSZ+99b]. **Propagation** [SGB16]. **Propagator** [CTCS05, CO17, GEO91, Lon99, Löw85c, MM96, Odd78, ÖB81, Yea05, ZDZO11, Lin02, Öhr02, Ort22]. **propensity** [Hes22]. **Properties** [ABB90, BMPV99, BU97, BJMB14, BK70, CTS04, CCCC15, CMVPFC16, DO09, DA14, DST+03, FE97, Fuk00, GVFG09, Hal64, JJD05, KsKsN08, Kla81, Kot68, KKGG98, Kry81, Kry03, KO19, LDB95, LHL18, Lon99, Löw96b, OK11, OBHM17, PV09, Rei73, RM04, She15, TY85, UK05, VWP+98, Wei72, Bis19, RSP21, SBLJ05, TM21]. **Property** [FPL97, MWL+05, Nic11, Nic17, SB99, SYIY03]. **Property-Specific** [Nic11, Nic17]. **Prospects** [WM97]. **Protein** [GBPSR10, FB20, GG20, LL20]. **Proteins** [Kot68]. **Proton** [BWVD+13, Coo18, CS04, DBC+99, HSS+04, McG04, MBM99, Oni15, PBK04, SIY+15]. **Proton-Conductors** [Oni15]. **Protonated** [KKK+97]. **Protonation** [PWZ+08]. **Protons** [AGMdV+13, BRL13, CTSDÖ05, AA19, Kar24]. **Pseudo** [CKRT03, DST+03, GW17, KBS03, TSTH03]. **pseudo-binary** [TSTH03]. **Pseudo-Jahn** [CKRT03, DST+03, KBS03]. **Pseudopotentials** [Gut97]. **PSII** [YKS+12]. **Pt** [SN08, Hog18e, KBH23, KC19, SH19, WHB+24]. **Pt/Al** [KBH23]. **publications** [Ano04i]. **puckering** [MFMCN01]. **Pulse** [VTM98, CM24]. **Pulsed** [BS98]. **Pulses** [MCP12, ML18]. **Pure** [Gal73, LK90, MLR+98]. **Pure-State** [LK90]. **Purine** [PP68]. **purpose** [LH20]. **Pyramidal** [YTC+05]. **Pyrimidine** [PP68].

QED [LT98]. **QM** [BBB10, MC10, SBC10, SIY+15, TL10, ZLC+10]. **QM/MM** [BBB10, SIY+15, MC10, TL10, ZLC+10]. **QSPR** [Sey12]. **Quadratic** [BB13, GC92, LPDB03]. **Quadrature** [Kou15]. **Quadrupole** [PS05a]. **qualitativeness** [PB20a]. **Quantification** [Bel06]. **Quantisation** [PS05b]. **Quantitative** [WD70]. **Quantities** [CH03, KTC01]. **Quantum** [AČP88, AT91, And80, Ano04l, Ano13a, Ano13b, Ano19a, AA01, AGL05, BND81, Bad09, BR82, Bel09, Bel11, BSB13, BB17, BR17, BR65, Brä08, BR20, Brä21a, BB22b, Brä22, BB24a, BKB+19, CCM05, CL05, CD05, CCVB94, CCC17, CS77, CC97, CB18, Cra99, Dau67, Dau70, DO09, Deu99, Dra20, DKV+19, DW98, Fro02, GC10, GG20, GMB04, GSWW10, HPL98,

HG17, HPRR10, Hog13a, Hog13b, HB14, Hog18b, Hog18e, Hog21, Hog23a, Hog23c, HDFT24, IBB+19, ILS08, Jan65, JKMB19a, Kar97, KS97b, KBH23, Kla81, KD11, Kra99, Kuk14, KV08, KZR86, Lad73, LBH+17, Lar17, Len68, Löw64a, Löw65a, Löw65c, Löw67a, Löw67c, Löw68a, Löw70a, Löw72a, Löw73a, Löw74a, Löw75a, Löw77a, Löw78a, Löw80a, Löw81a, Löw81b, Löw82a, Löw82b, Löw85a, Löw86a, LSZ88]. **Quantum** [LSZ89, LSZT90, LSZ91, LSZ92a, LSZ92b, Löw92a, LSZ94, LSZ95, LSZ96, LSZ+97b, LSZ+97a, LSZ+98b, LSZ+98c, LSZ+98a, LSZB99, LSZ+99b, LSZ+99a, LSZ+00, LSZB00, LL20, MG21, MCG+08, MS03, MG20, Mat64, McW98, Mez96, MT04, Mic17, Miy03, Moh98, Moh08, MP97, MG23a, NAY+08, NFW+98, NBS10, Nic11, OS05, Öhr17, Oni12, Oni15, PD10, PBOL02, PSAP10, PB20c, Pul77, Pyy78, QSG98, Ray95, Ryc98, SBM+01a, SBM+01b, SB02, SBA+03, SB03, SBC+03, SBCT04a, SBCT04b, SBK04, SO05b, SB05, SBLJ05, SB06, SB07, SBSL08, SBK+08, SBGJ08, SBC09b, SB09a, SBC09a, SBC10, Sab11, SB11, SB12a, SB13a, Sab15, SB17a, SB18a, SPD09, Sal11, SJO05, Sey12, Sig05, SBG+98, SAL10, SGK+08, Sut98, TMN10, Tap09, Tap11, Tap17, TR14, TMMS10, Tos08, TL10, VTM98, Wei72]. **Quantum** [WMM+98, WDD16, vS07, BMR+24, BPK23, BP20, BKL21, CCT02, EW03, HO16, Kar24, LÖS02, LT21, Mic02, MOB+03, NBA20, NTT20, Per20, PMK23, SB17b, SH19]. **Quantum-Chemical** [Kuk14, SJO05, PBOL02]. **Quantum-Classical** [MT04]. **quantum-electrodynamic** [PMK23]. **Quantum-Informed** [TR14]. **Quantum-Mechanical** [BB17, KZR86, Pul77, Wei72, vS07]. **Quantum/Classical** [GMB04, PSAP10, EW03]. **Quarks** [JL03]. **Quartet** [ZBM98]. **Quasi** [GDL14, JSG+14, Shi12]. **Quasi-Bound** [Shi12]. **Quasi-Molecule** [JSG+14]. **Quasi-Newton** [GDL14]. **Quasidegenerate** [BB99b]. **Quasiparticle** [HL90]. **Qubits** [Coo18]. **Quest** [PM14]. **Questions** [DE05].

R [HSR98, JJD05]. **R.** [AGS+19]. **Radial** [ÖÖ13, PS05a, SJO05, ALA23, Lin02]. **Radiation** [BWVD+13, BB13, BB15, Bic13, CL07, CT82, Glu19, LS07, PGJ07, Ram98, Sab07, Sal11, ST07, VTM98, SB07, SS22]. **Radiation-Induced** [Sal11]. **Radiationless** [OO82]. **Radiative** [BS98, BKB+19, DKV+19, KSG08]. **Radical** [ARS99, CL07, EEL96, KBS03, LM97, Lin05, LGK+99, She15, vS07]. **Radicals** [GAI08, LS07, MLPD+98, MVL01, RRMAF08, Tur07, VKI97, YMI+21]. **Radioactive** [Per98b]. **Radiobiological** [BB15]. **Radiobiology** [Fra13]. **Radium** [Bar23]. **Raman** [CM24, MCP12, TP03]. **Ramsey** [PB05]. **Range** [BBB10, Dru78, DB01, DB13, JGCRC16]. **Ranges** [AGO07, Pau13]. **Rare** [BG73, Jan65]. **rate** [SS22]. **Ratios** [MTA00]. **Ratner** [SB17b]. **Ray** [Ada00, CS77, GM17, Kaw97, KsKsN08, KNM+08, MYW00, MW08, MKK+00, MTA97, MTA00, Mur08, Tak19, Uda00, UMD08, YFK+97, Mur03, YKS+12, YNNU03]. **Rayleigh** [BH24, MM99]. **Rays** [AAM04]. **Rb**

[BJMB14]. **Re** [LSZ+99a]. **Reactants** [ASGG08]. **Reaction** [ACC99, ACDV01, ASGG08, BRW08, FHHZ88, Hog18e, JGNJ08, PL98, PTLGOM12, RRMAF08, Saa01]. **Reactions** [BR82, FF72, GAI08, HB14, Kuk14, MÅ01, MM99, MBM99, PSAP10, RAR+08, SW81, Sko12, TMN10, Hes22, PEMC23, YMI+21]. **Reactive** [GSWW10, Nal06]. **Reactivity** [Bro98a, Bro98b, Dau67, Dau70, MF14, MNR+98, Nal03, ST78, SH95]. **Real** [Ste73, Bis19, WLM23]. **real-time** [WLM23]. **realise** [Zap01]. **Rearrangement** [KS88, Mic99, UYT97]. **Reasonable** [WD70]. **Recognition** [Rei73]. **reconstructions** [BB22a]. **Recurrence** [BL18, ÖÖ13]. **Reduced** [BK70, Kry81, LGJP99, PKYM01]. **Reducing** [YÖ13]. **Reduction** [AHPD+03, OO05, OM03]. **Reference** [BŚG14, LT98, MDBM98, OB23, SH19]. **Refined** [YKS+12]. **Reflections** [Noo09]. **Reforming** [Fuk08b]. **Reformulation** [Cio90]. **REG** [FSP23]. **REG-MULTI** [FSP23]. **Region** [BS98, CCC17, GWW19]. **Regioselectivity** [RGA99]. **Regression** [Löw92a]. **Regular** [And80, SR73, YZDM01]. **Regularization** [PSS98]. **Reinvestigation** [PB05]. **Related** [ACDK72, KTC01]. **Relation** [DGA18, Kry03, Sri01, VG22]. **Relations** [BL18, IL98, KNN17, Löw92a, ÖÖ13, SPM09, EW03]. **Relationship** [KB86]. **Relative** [HB14, Kou15]. **Relativistic** [Bar23, Coh04, DKV+19, ERC88, FAS+98, Glu19, HMH+18, HBT+00, Khe19, Ono00, Pyy78, QSG98, SED+98, UK05, VI01, YZDM01, GPEB21, Sau05a, WHB+24]. **Relativity** [Brä08]. **Relaxation** [Jør74, PSAP10, SPG+22]. **Release** [Ber14]. **relevance** [Bel21]. **Relevant** [ILS08, Tur07]. **Remarks** [Die97, Uda97]. **Removing** [Sim05]. **Renner** [BMP03]. **Renormalization** [Kri03, PSS98, RPSB00]. **Reorientations** [YAJHR03]. **Repair** [BB13, BB15]. **Repair-Based** [BB13]. **report** [Gos02a]. **Representability** [LK90]. **Representation** [DGA18, JSG+14, KT98, Per98a, SGB16, JS21]. **Representations** [CTG98]. **Reproduce** [DSW04]. **Reproduction** [KMR01]. **Repulsion** [Ave13, AA18]. **Repulsive** [DB01, DB13]. **Required** [JJD05]. **research** [Gos02a, KÖO23]. **Reservoirs** [Mar08b]. **Residues** [ST17]. **Resolution** [BB11, BB17, Jos08, YKS+12]. **Resolved** [WmG18]. **Resonance** [Bel06, BB11, DeB09, HBE+98, KG12, LA12, Löw88b, LFM89, Ram08, Vis05]. **Resonances** [MM96, Nic17, STZY18, SW81, Sko12, BB21, FCAG19, FTG22]. **Resonant** [AAE+01, GC10, GP04, KO19, PLA01, UYT97]. **Resonant-Coherent** [GP04]. **Response** [ÅVM96, BB13, FPL97, HJ99, JJD05, JH99, Krs16, LV90, LÅJM95, Mic15, MCA+18, PS05a, PM16, RTV05, SBLJ05, Sim05, BLC23, TM21]. **Rest** [KS88]. **Restricted** [FCH15, RTV05]. **resultant** [Nal23]. **Results** [BG23, BH24, Lad73, Miy03, VTPR97, VWOS89, WM97]. **Review** [ASGG08, DB13, Kla81, KHPP23, MK23, Nor98, PMK23, ZZ08, BPK23]. **Revision** [TAM04]. **Revisited** [BND81, BE04, Ran18]. **Revisiting** [LPC24]. **Rh** [GBHM14]. **Rhombohedral** [NP03]. **Rigged** [Tap01]. **Rigid** [Sme92].

Ring [CPBS05, MFMCN01]. **Rings** [FLV99, PWZ+08, BMC97]. **Ritchie** [AGS+19, SO19b]. **Ritz** [BH24, MM99]. **RNA** [AGO07, KN01]. **Robust** [Kou15]. **Role** [GAI08, Kap98, LA12, LASV18, TSON00]. **Root** [MH98]. **Roothaan** [DKMP98, OE17, ÖEO23]. **Rosen** [McW99]. **Rotation** [PR05, SR73, YTC+05]. **Rotation-Vibration** [YTC+05]. **Rotational** [Les75, MWL+05, SJO05, Sau05b]. **Rotations** [CMDN89, MFLK11]. **Rototranslational** [LDB95]. **route** [Hog23c]. **Routes** [BBB10]. **rubrene** [ZLL+20]. **Ruby** [ITI+00, OYI+00]. **Rufus** [SO19b]. **Rule** [CTSOS99, KP77]. **Rules** [CTO18, Coh04, LDB95, OOSS17, Yan81, CTSSO19]. **RuO** [NIO03]. **rutile** [Sak03a]. **Rydberg** [LM97, MLPD+98, MVL01].

S [CSZ99, Miy03, MFMCN01, VT24]. **Sabin** [OB22a]. **Salpeter** [ORL23]. **salt** [MST+03]. **saltatory** [JJ20]. **Sampling** [HS19]. **Sandwiched** [OBHM17]. **Satellite** [Uda00]. **Scalar** [CPBS05]. **Scale** [Fra13, SIY+15]. **Scaled** [STZY18]. **Scaling** [Lev90, Löw88b, LFM89, LLBK+98]. **Scattered** [HL97, Joh73]. **Scattered-Wave** [HL97, Joh73]. **Scattering** [GSWW10, Nes75, Shi12, ST07, TP03, WHB+24, AMAA22, BKL21, HHU+21, HM19, Kar24, SJAB+22]. **ScB** [KM98]. **SCC** [dLHD10]. **SCF** [Ave98, CG80, CDP82, GVFR98, PTC+13]. **SCF-LCAO** [PTC+13]. **Scheme** [DKMP98, LFM89]. **Schemes** [MC10]. **Scholar** [SO19b]. **Schrödinger** [MKN10, BG23, Hyl64, MFCT15, SBK15, VTPR97]. **Science** [JG08, McW01, Odd05, Tan00, AO03, LSZ+00, SBA+03, SBGJ08]. **Sciences** [Löw92a, Ram08]. **Scientific** [Bun17, Kar02]. **Scientist** [Lin99, OB22a, Öhr05]. **Scope** [SIY+19]. **Screening** [HL90, MA04]. **Search** [Kom05, Lev90, Löw92a, Nes98, Zap01]. **Searches** [Kar08]. **Second** [AHPD+03, HJ99, Hät05, IL98, LDB95, MW98, RR05, SW98]. **Second-Order** [Hät05, IL98, LDB95, RR05, SW98, AHPD+03]. **Section** [Jos08]. **Sections** [CTSDÖ04b, CTSDÖ04a, HMH+18, PBK04, RGFC13, MG22]. **Selected** [Bun18, CHSC03, Mar08a, CAG+21, SM22]. **Selection** [CTSOS99, HS19]. **Selective** [AAM04, KKA97, LGK+99, MM99]. **Selectivity** [RGA99]. **Self** [DDPC95, GDL14, HL90, LJKH13, LSC19, Per90, Sla72, WD70, YNNU03, Ort22]. **Self-absorption** [YNNU03]. **Self-Consistent** [GDL14, Sla72, LJKH13, LSC19]. **Self-Consistent-Field** [WD70, Ort22]. **Self-Energy** [DDPC95, HL90]. **Self-Interaction** [Per90]. **selforganization** [Brä02]. **Selftrapping** [MS03]. **Semi** [HSS+04, LK09, Sim99]. **Semi-Classical** [Sim99]. **Semi-empirical** [HSS+04]. **Semi-infinite** [LK09]. **Semiclassical** [HPU+17]. **Semiconductor** [Kra99]. **Semiempirical** [HPU+17]. **Seniority** [ATL+18]. **sensitive** [AMAA22]. **Sensitivity** [PM14]. **sensitized** [GTB23]. **Separability** [McW98]. **Separation** [DeB09, OYI+00]. **Sequence** [CÅ01, VI01, VT24]. **Sequences** [KGW98, KCM70, VT24]. **Sequential** [CCM05, CC97]. **Series** [Ano08l, Ano09i, Ano12h, Ano14e, Ano15g, Ano15h, Ano16d, Ano17j, Ano17k, Ano17l, Ano18d, Ano19q, Ano19r, Ano20g, Ano20h, Ano21g, Ano21h, Ano22h, Ano22i, Ano23g, Ano23h,

Ano24d, CB18, Hog18f, Jør78, PB75, SB13e, BG23, SÁ23a]. **Set** [CTSOS99, QGW01, SDGW98, Tap17, VWP+98, RA19, SKGŚ23, Wen21]. **Sets** [AT91, AH19b, GW01, Kla81, MW98, OOSS17, PTC+13, QGW01, SPAS05, SW98, VWP+98, WM97, CCM+19, CAP19, GW23]. **Seven** [HDFT24, LC03]. **Shakeup** [SNMI00]. **Sham** [GV09, KB98, LK90]. **Shape** [AMAA22, MM96]. **Shape-sensitive** [AMAA22]. **Shapes** [BWK97]. **Shell** [Bra77, CG80, DKMP98, FMA08, GVFR98, HUS+11, HL97, JSF08, KS88, LP97, LASV18, MP89, RTV05, MU03, VG22, YMI+21]. **Shielding** [JH99, JcH18, Vis05]. **Shift** [AB73, NA19]. **Shifts** [DY08, HDB03, PGV97]. **Short** [DB01, SGB16]. **Showing** [Jør74]. **SI** [Moh08, CTSSO19, JS21]. **side** [BFHS23]. **Sightseeing** [Ros98]. **Sign** [NA19]. **Signal** [BB11, BB17, DeB09]. **Signal-Noise** [DeB09]. **Signals** [Bel06, Bel11, BB22a]. **SiH** [JSG+14, MVL01]. **Silicate** [KE97, KE00]. **silicates** [NHM03]. **silicide** [TSTH03]. **Silicon** [DO09, HOI+08, KIHA97, EOH03]. **Similarities** [MVL01]. **Similarity** [CCVB94, Löw88b, LFM89, SNM+97, WN05]. **Simple** [AČP88, San98]. **Simplest** [SGM+13]. **Simplest-Level** [SGM+13]. **Simulate** [JJD05]. **Simulation** [Fra13, HB14, MP97, RFG+98, MFMCN01]. **Simulations** [BHV+00, CMJR+04, GBPSR10, HS19, HBGvM19, PWZ+08, TMN10]. **SiN** [Jan97]. **Sinc** [Kou15]. **Single** [BRL13, Bis67, EM17, GWM+03, HBE+98, MH98, Nag01, Tos08]. **Single-** [EM17]. **Single-Center** [Bis67]. **Single-Root** [MH98]. **Singles** [HS86, LGJP99]. **Singlet** [BHM17, GV09, GL68, RLF17, Sme99, SKS+19, VT24]. **Singlet-Triplet** [GL68]. **Singularity** [GS04a]. **SiO** [GP14, MKK+00, OTA97]. **Site** [Bro98a, Chi03, Bro98b, DAB+23]. **Situation** [OW08]. **SIWB** [Fuk15]. **Six** [BH24]. **Size** [CDK15, DDPC95, EM17, IKN+08, Per90]. **Size-Consistency** [DDPC95, Per90]. **Size-Extensivity** [EM17]. **Size-Intensivity** [DDPC95]. **Sizes** [LR72]. **Slag** [MKK+00]. **Slags** [MKH+97]. **Slater** [AYÖ17, HPB17, KÖO23, Mon05, PTC+13, PTBH13, Rui23]. **Slater-Orbital** [Mon05]. **Slater-Orbital/Plane-Wave** [Mon05]. **Slater-Type** [AYÖ17, HPB17, Rui23]. **Slow** [SCTH+07, JS21]. **Small** [HL97, Kap98, Nes67, RK04, UK05]. **SMILETRAP** [SBF+08]. **SnO** [GP14]. **Sodium** [CKRT03, NHM03]. **Soft** [AAM04, KNM+08, Mur08, UMD08, Mur03]. **Software** [KS97b]. **Solar** [KD11, GTB23]. **Solid** [AYÖ17, AJ04, EG99, FAS+98, Löw65c, Miy03, SR73, IOA03, SEL01]. **Solid-State** [EG99, IOA03]. **Solids** [AL04, CMJR+04, DC99, GSTvE98, Gon98, GL90, Köv08, PGN04, AP03, AGS+19, MAS03, SSK03]. **Soliton** [För94]. **Solution** [BH24, BE01, Cam12, CCM05, CB18, JGCRC16, KGW98, MYW00, MFCT15, MKN10, PWZ+08, dLHD10]. **Solutions** [BC09, HPRR10, Kob97, TMN10, MST+03, SKGŚ23]. **Solvation** [KGW98]. **solvatochromism** [CCT02, LCC22]. **Solvent** [AB73, ABC+98, BMPV99, Bas64, CC97, GMLSC+10, MBM99, SS22].

Solvent-Mediated [MBM99]. **Solvent-Shift** [AB73]. **solvents** [CCT02, LCC22]. **Solver** [BS05a]. **Solving** [YÖ13]. **Some** [Ber74, CG80, Dau70, DE05, GEO91, HPB17, HKS90, Ler85, Löw85c, LM92, Löw96b, Löw98, STZY18, SGM+13, Sut98, Sut01, UK05, VTPR97, WM97, YFK+97, SBC10, Löw65c]. **Son** [Heh18]. **Source** [GDL98, Lyo08]. **Sources** [AVB08, BGG+07]. **Space** [BB99b, Dah01, FCH15, GW17, GSWW10, LEK01, MMSK16, Bis19, LMK19, ÖEO23, TMK21]. **Space-Pseudo-Time** [GW17]. **Spaces** [LK09]. **Spatial** [ATL+18, BLC23]. **Special** [Ano12i, Brä08, Löw85c]. **Species** [DNM+14, She15]. **Specific** [Kar24, MDBM98, MKN10, Nic10, Nic11, Nic17]. **Specifics** [Bun17]. **Spectra** [ÅCL92, Ada00, AB73, Bas64, Bas78, Bel11, BB99b, CÅ01, HDB03, JJD05, JGCRC16, Jør74, Jør78, Kaw97, Köv08, Löw88b, LFM89, MVL01, MC10, MHWvdA97, NM00, NBS10, Pet98, RLF17, SJO05, SSV98, Tak19, Uda00, EÜSB21, IOA03, Köv03, Mur03, NBS12, Sak03a, SA23b, YNNU03]. **Spectral** [APNM03, BS98, Mur08, OO05, PB75, UMD08, YKY+00]. **Spectrometer** [KNM+08]. **Spectrometric** [MRS+99]. **Spectrometry** [OO05]. **Spectroscopic** [JJD05, LvWH+01, MW08, RM04]. **Spectroscopy** [BBB10, Bel06, BB11, BB17, BS98, BKB+19, CE78, DKV+19, DeB09, Glu19, HSS+04, Hug98, ILS08, KGI+19, MYM08, Per98b, Ram98, Ray95, SCM09, BB21, BB22a, LSZ+00]. **Spectrum** [Ada97b, CCCC15, CSZ99, MKK+00, SP99]. **Spherical** [Aqu09, Dol09, Lau09, Lin17a, PS05b, SR73]. **Spheroconal** [MFLK15]. **Spheroidal** [KO18, MFA21]. **Spin** [ÅVM96, CAG+21, CHSC03, CCSZ01, DAB+23, DE05, ERC88, Gal73, KKA97, LP97, LF09, Lon99, Mat64, May80, MÅ01, NeMM03, PKYM01, RM04, RP72, Sal74, SPAS05, Sau05a, WmG18, YKS+12, Yea05, Fuk03, VT24]. **Spin-adapted** [CAG+21]. **Spin-constrained** [DAB+23]. **Spin-Coupled** [CCSZ01]. **Spin-Crossover** [NeMM03]. **Spin-Free** [Mat64]. **Spin-Interactions** [Sau05a]. **Spin-Orbit** [ÅVM96, ERC88, LF09, RM04]. **Spin-Projected** [May80]. **Spin-Resolved** [WmG18]. **Spin-Selective** [KKA97]. **Spin-singlet** [VT24]. **Spin-Spin** [DE05, Lon99, PKYM01, SPAS05]. **spin-states** [Fuk03]. **Spin-Tensor** [Yea05]. **Spins** [Eks98]. **Square** [Löw92a, MFCT15, YFK+97]. **Square-planar** [YFK+97]. **Squares** [LJK+08]. **Squeezing** [BR17, Phi98]. **Sr** [GWM+03, KIT+08, GVFG09, NIO03]. **Stability** [Eks98, Jan97, Jan65, MBAPS19, TLOK97, CBSM20, FB20, YIYM03]. **Stabilization** [SSS05]. **Stacking** [FU00, UJYU03]. **Standard** [LBH+17, CCM+19]. **Standpoint** [vS07]. **State** [Ada97a, AdMB99, AB73, AH19b, BS04, CMVPFC16, EG99, Fuk08a, HBKS03, KT15, Kom05, KE97, LT98, LPDB03, Lin98, LK90, MDBM98, MS03, MKN10, MW98, MKK+00, Nag01, Nic10, Nic11, Nic17, RLF17, RT18, Tap17, VWOS89, WMM+98, WN05, CTSSO19, CBSM20, Dur20, Hog21, IOA03, MFMCN01, NHM03, RA19]. **State-** [Nic11, Nic17]. **State-Quantum-Chemistry** [Tap17]. **State-Specific**

[MDBM98, MKN10, Nic10]. **States** [AAE+01, ALND10, AR03, AA05, BR05, BK70, CY00, CKRT03, FE97, GAI08, Gal73, GC10, GV09, Hät05, KM98, KG12, Kom05, KE00, KO19, LMSP01, LP97, LA12, LKD05, Löw88b, LFM89, MKN10, MKH+97, MYM08, MMSK16, Nag97, Nic10, Nic17, Oli90, PD10, PB99, RPSB00, RAR15, RM04, Shi12, Sme99, SBDD03, Tap11, TM13, Wei04, Bel19, BKL21, Fuk03, JMWG19, MFA21, MK23, Nag03, Nal23, NBS10, NBS12, OTA03, OB23, PS21, SZP21, UJYU03, VT24]. **Static** [IS01, PM16]. **Statistical** [Kou15, PD10, Sla72, Spe78]. **Status** [Bun18, KT15, SBG+98]. **Steam** [Fuk08b]. **Steel** [MKH+97]. **Stemming** [YZDM01]. **step** [HDFT24, RZTSW23]. **Stereochemistry** [CH03]. **Stereoregular** [CMFA99]. **Stereoselective** [LDP+04]. **Sternheimer** [FPL97]. **Sternheimer-Like** [FPL97]. **STO** [AA18]. **Stochastics** [Bic13]. **Stoichiometric** [APNM03]. **Stopping** [AGO07, BS04, CTSDÖ04a, CTSO04, CS04, MTS04, McG04, NA04, PGJ07, Pau13, PBK04, Por04, SO05a, SRZE04, Sig05, CTO22, MMM22, MG22, VG22]. **Storage** [PB14, YM97, YM00]. **Stored** [Ber14]. **STOs** [LPC24, ÖÖ13]. **Strand** [Sim07]. **Strategy** [CTG98]. **Strength** [CTSO04, HK03, OOSS17, TLOK97, CTSSO19]. **Strengths** [BLKS78, CTSOS99, Khe19]. **Stretching** [She15]. **Strong** [Chi03, DKV+19, IS01, SBG+98, VTM98]. **Strongly** [DBC17]. **Structural** [DO09, MYW00, SIY+19, VWOS89, YKC+08, Yam03]. **Structure** [ADRAB16, AH19b, Bli65, CL00, DLMS03, EGCL91, EEL96, FP06, FCH15, Fuk00, Fuk15, GSTvE98, GS04a, Gre08, GM91, Har18, Hät05, HJ88, Hog13g, IOI+00, Jan97, KM98, Kat03, Ker82, KsKsN08, KIHA97, KNI+08, KSY08, Kot68, Löw80b, LASV18, MYW00, Nal03, OYI+00, PGN04, PWZ+08, PP68, SS98, SPD09, ST78, SMAS08, TY85, TS10, WD22, YFK+97, BKL21, CTO22, CCL03, EW03, GTB23, Hog14, Ito03, KC19, LSZ+97a, LSZ+99a, LSZB00]. **structure-function** [EW03]. **structured** [Mur03]. **Structures** [BMPV99, CMVPFC16, HOI+08, HTS+00, ITI+00, KIT+08, Köv08, KN01, SNM+97, SIY+19, SSV98, SNIM08, Uda00, YKS+12, YM00, EOH03, KOT+00, KTA03, NHYU03, NIO03, YIYM03]. **Strutinsky** [DKMP98]. **Studied** [BRW08, HSS+04]. **Studies** [AAE+01, AA19, ASGG08, BWH08, Cse97, DY08, Fra13, FHHZ88, Gre73, Les75, LM92, LGK+99, MCG+08, Mar08b, MW98, RAR+08, Sab07, Tur07, MGAUP23, PBOL02, RSP21]. **Study** [ARS17, BJMB14, CTCS05, CCM05, CG80, CL07, CKC09, CPBS05, CS77, CSZ99, Cru09c, DO09, DNM+14, GMLSC+10, GV09, GBHM14, ILS08, JJD05, Jan97, JGCRC16, KIT+08, KGW98, KB98, KKA97, KT98, Lad73, Mam19, MYW00, MW08, MBM99, PSAP10, RMN+14, RRMAF08, RT18, Sab97, SG80, VKI97, YFK+97, ZBM98, BMC97, Bel19, BTB+20, GC01, ORL23, TBM01]. **Sturmian** [AA01, AAG03, AAAC04, GAM+13, GW23, GCAGM17, KO18, MFA21, RA19]. **Sturmians** [Ave98, AA05, Ave13, AA18, CCA13, Gos02b]. **Subject** [Ano64e, Ano65e, Ano67f, Ano68f, Ano70f, Ano72f, Ano73f, Ano74d, Ano75d, Ano77e, Ano78d, Ano08m, Ano12j]. **Subshell** [KRL01]. **Subshells**

[HMH+18]. **Subspace** [GDL14]. **substituents** [GC01]. **Subsystems** [Nal00]. **successive** [PEMC23]. **Sulfur** [SN08, TSON00]. **Sulfuric** [BWH08, KLG+08, KV08]. **Sum** [CTSOS99, CTO18, Coh04, LDB95, OOSS17, CTSSO19]. **Summary** [Lad73]. **Summation** [SÁ23a]. **Summations** [DDPC95]. **Super** [KE98]. **Super-Heavy** [KE98]. **Superconducting** [TMM03]. **Superconductivity** [DB13, DBC17, Kri03]. **Superconductors** [DB01, Lar17]. **Supercritical** [CCCC15, CCC17, Gre08]. **Superexchange** [MCC03]. **Superheavies** [Gre08]. **Superheavy** [FSB+97]. **Superionic** [KTMA08]. **Superposition** [Tap09, VWP+98]. **Support** [Duc97]. **supported** [Hog23c]. **supporting** [Per20]. **Surface** [IKN+08, LC03, PGN04, SN08, VWOS89, Sak03a, SH19, SHBC19, SKK23, ŻM23]. **Surfaces** [AJ04, BB99b, BWH08, LBH+17, SS98, TTLB04, AGS+19, HM19, SCE19, Tők19]. **Surrounding** [Jør74]. **survey** [Ros97]. **Susceptibility** [Laz04]. **Suter** [Miy03]. **Swift** [Sab97, SBCT04a, SBCT04b]. **Switching** [ST17]. **Symbols** [McW01]. **Symmetric** [ACDV01, Col68, Gal73]. **symmetries** [QSW20]. **Symmetry** [AAM04, Ber03, BK70, DST+03, Fow03, Har05, KCM70, KMJ97, Kry81, Ser74, SBDD03, Yan81, KHPP23]. **Symmetry-Adapted** [KMJ97, KHPP23]. **Synthesis** [LDP+04]. **System** [CDK15, GVFR98, Mic15, Moh08, SIY+15, Tos08, ZBM98, Mic22, ŻM23]. **System-Size** [CDK15]. **Systematic** [BJMB14, KGW98]. **Systematically** [SW98]. **Systems** [APNM03, AČP88, ABB90, AGL05, AK12, BGG+07, Bad09, BS72, Ber03, Bra77, BC09, Cal85, CB18, DKV+19, DR90, DBC17, EG99, FIK+03, Fow03, FCH15, Gal73, GC10, HS05, HA13, Har17, HG17, HMW01, IBB+19, KS77, KT98, KTC01, KNN17, KGI+19, LPDB03, LS07, Lin17a, Lin17c, Mar08a, MC10, McW98, MT04, Mon05, MBO+07, Nal06, Nal09, Ohn67, PČ75, PKYM01, Pol03, RTV05, RAR15, RLF17, San98, SRZE04, SPM09, Shi12, SCM09, Sut98, TY85, TAM04, WDD16, BLC23, BPK23, Brä02, KC19, LSZT90, LSZ+98b, LSZ+98c, Min22, SBM+01a, SBM+01b, SBC09b, SBC09a, SPG+22, TSTH03].

T [DB01]. **taa** [NeMM03]. **taatris** [NeMM03]. **Table** [Ros98]. **Target** [CTSO04, CTO22]. **Targets** [CS04, HMH+18, MMM22]. **Tartaric** [HSR98]. **Tautomeric** [KZR86]. **Tautomerism** [KN01, LK14]. **Tautomerization** [HBGvM19]. **Teacher** [Öhr05]. **Teaching** [Deu99]. **Technique** [Löw67c, Löw98, WD70, Lar02, MG21]. **Techniques** [CCVB94, DSR81, Eks98, Mon05, PB75, BPK23]. **Teller** [ABGM03, ADA03, BP82, BO86, Ber03, BMP03, Chi03, CKRT03, DST+03, FIK+03, GWM+03, HBKS03, KH03, KBS03, LPDB03, LC03, LM03, MS03, MCC03, NeMM03, OM03, Pol03, SKT+03, SS03, SIY+19, SCN03, YAJHR03]. **Temperature** [DLMS03, DB13, DBC17, HK03, HBKS03, MF14, WDD16, TMM03, TSTH03, ZLL+20]. **Temperatures** [BB14, Sak03b]. **Tempered** [KGW98]. **Tensor** [MWL+05, Sau05b, Yea05]. **Tensors** [JcH18, Vis05]. **Term** [AHPD+03, VI01, BMR+24]. **Terms**

[BVHK03, Jan65, Kho04, NM03, Öhr16, PKYM01]. **terpenes** [Hes22]. **testing** [PEMC23]. **tetraazacyclotetradecane** [MYW00]. **Tetragonal** [DA14]. **Tetrahedral** [CL05, Cse97]. **Tetramethyldiamide** [HSR98]. **tetraphenylporphyrins** [NHYU03]. **Tetroxide** [RNL14]. **Their** [AČP88, AFE13, BWK97, FE97, GDL98, HM21, KNM+08, LA12, PP68, RK04, Sva98, TY85, dLHD10, Hes22, KOT+00, SYIY03, VG22]. **theorem** [Ort22]. **Theoretic** [Kob68, Nal03, Nal23]. **Theoretical** [Ada97b, Ada00, ASGG08, BWH08, BKC68, BTB+20, CCVB94, CPBS05, CSZ99, DSR81, FHHZ88, GM05, IFAY08, JJD05, JG08, KP77, KKK+97, LK14, Ler85, LGK+99, MG21, MST+03, Miy03, MAS03, MHWvdA97, Pet98, RAR+08, Sab07, STZY18, SIY+15, SIY+19, SG80, Sla81, SSK03, TBM01, ZZ08, ZBM98, Brä03, GC01, SBGJ08, SL20, SEL01]. **Theoretically** [Mur03]. **Theories** [BMM13, Bra67, Cio90, DB68, FH65, GL90, LK13, Nag03, WN05, Bel22, LH20]. **Theorists** [Len68]. **Theory** [ÅVM96, ÅCL92, Ano04l, ARS17, ACDK72, AGL05, BND81, BVHK03, Bas64, Ber74, Bli65, BC00, Brä08, Brä12, Bra77, Bro98a, Bro98b, BŚG17, CTS04, CTCS05, Cam12, CG80, CDP82, CCSZ01, CO17, Dau67, Dau70, Del74, DC99, EG99, EEL96, FP06, FF72, Fuk15, GC10, GC92, GW17, GDL98, GBHM14, Gon98, GS04a, GSWW10, GS04b, GK90, Gut06, Hal91, Har90, Har67, HJ99, HJ88, HBE64, Hog13g, HW01, HMC73, Joh73, Khe19, KMHL13, KMJ97, KK85, KB86, Lad73, Lau09, Lev90, LP97, LS03, Lin17c, LJKH13, LB92, Löw65c, Löw67c, Löw88b, LK90, LLBK+98, LÅJM95, MH98, Mat96, MS65, MFLK15, Mic15, Nag97, Nal09, NSM11, Nes75, Nes03, Nic10, Nik70, Noo09, ODE75, ÖB81, PČ75, Pal04, Per90, PB05, PM16, PGP17, RR05, RTV05]. **Theory** [RC05, SBCT04a, SBCT04b, SB07, SBC09b, SBC09a, SRZE04, SS03, SS90, SW98, Sid18, Sig05, Sme92, SGM+13, TMN10, Tap01, Tap09, VWOS89, VKI97, VRG90, VI01, WT99, Yan81, Yan90, AO03, CTC22, CBSM20, GTB23, HM19, KHPP23, LSZT90, LSZ+98a, MGAUP23, MPU19, MOB+03, MK23, NBS12, OB23, ÖEO23, PEMC23, PMK23, SBLJ05, Tew21, TM21, Zap01]. **Theory-based** [SRZE04]. **Theory-The** [Gut06]. **Therapy** [BWVD+13, Bic13, PGJ07, Pau13, Bel21]. **There** [FCC04]. **Thermal** [MYM08, TLOK97]. **Thermochemistry** [Hur73, Mar08b]. **Thermodynamic** [CCC17]. **Thermodynamics** [HBGvM19, Spe78]. **Thermoelectric** [SNIM08]. **Thickness** [IKN+08]. **Thin** [KsKsN08]. **thiol** [GC01]. **Thiouracils** [KN01]. **Third** [BB99b]. **Third-Order** [BB99b]. **thirty** [Ros97]. **Thomas** [CTC22, Cru09c]. **Thoughts** [Bic04, HKS90]. **Three** [AAE+01, CM24, CB18, GAM+13, HA13, Jan65, Ros98, BKL21]. **Three-** [HA13]. **Three-Atom** [Jan65]. **Three-Body** [AAE+01, GAM+13, BKL21]. **Three-Ion** [Jan65]. **Three-Particle** [CB18]. **Threshold** [MFCT15, AA19]. **thymine** [SS22]. **Ti** [CL00, FU00]. **TiC** [SNM+97]. **Time** [ARS17, BBB10, Bel06, Bel11, GW17, GK90, HG17, JGCRC16, KMHL13, LHL18, Lin17c, Löw67c, MKN10, MCA+18, Öhr15, Öhr17, PČ75, PR98,

PS21, SGB16, VTM98, WT99, BB22a, LSZ+99a, LSZB00, NA19, WLM23]. **Time-Dependent** [ARS17, BBB10, GK90, HG17, KMHL13, LHL18, Lin17c, Löw67c, MKN10, MCA+18, Öhr15, Öhr17, VTM98, WT99, PS21, LSZ+99a, LSZB00, NA19, WLM23]. **Time-Independent** [BBB10, PČ75]. **Times** [TMMS10]. **tin** [GWW19]. **TiO** [GP14, Sak03a]. **tissue** [Per20]. **titanium** [TSTH03]. **TKHS** [DLMS03]. **Toluene** [RAR+08]. **Tool** [VKI97]. **Top** [Oli12]. **topics** [SBA+03]. **Topological** [Sjö04, JJ20]. **topological-homotopy** [JJ20]. **Total** [AGO07, CTSSO19, CTC22]. **Tour** [Ros98]. **Tracks** [Fra13]. **tragicomedy** [SL20]. **trail** [AGS+19]. **Trajectories** [GMB04, PSAP10]. **trans** [För94]. **trans-Polyacetylene** [För94]. **Transfer** [BMM13, CHR13, CCSZ01, DBC+99, FLV99, KKA97, LJ17, Les75, MBM99, OYI+00, SIY+15, Lar02, TBM01]. **Transferability** [ODE75, SKK23]. **Transferable** [KTC01]. **Transform** [Bel06, DeB09, HPB17, Mon05, ÖÖ13]. **Transformation** [LLBK+98, PTBH13, RZTSW23, TSTH03]. **Transformations** [CDP82, Löw88b, LFM89]. **Transformed** [WN05]. **Transforms** [AYÖ17]. **Transition** [Ada97a, ARS99, DLMS03, EGCL91, GAI08, HS19, Lin98, MCC03, RR05, SED+98, TLOK97, VI01, AO03, FCAG19, FTG22, MU03, TMM03, Yam03]. **Transitions** [GL68, HK03, LM97, MCP12, MLPD+98, Nik70, BSL+19]. **Translation** [SR73]. **Transmission** [BR05]. **Transport** [BR05, GG20, MOB+03, Rou20]. **Trapped** [WMM+98]. **Trapping** [Phi98, RDNFH98]. **Treated** [Bad09, Löw67c]. **Treating** [NBA20]. **Treatment** [BMPV99, BWVD+13, HL90, Kar97, Kho04, KTC01, LS07, LR72, Lin98, MTS04, Mic99, Nic17, Öhr15, Oli90, PKYM01, VTM98, MKK+01, PMK23]. **Treatments** [ATL+18]. **Trends** [BJMB14, UK05, HPL98, KÖO23, SBSL08]. **Triatomic** [BR82, Pet98]. **Tribute** [SBK04, LSZ+99b, SB02, SBLJ05, SCT15, SCT16]. **Triggered** [Kuk14]. **Trigonal** [ITI+00]. **Trioxide** [SN08]. **Triples** [BB99b, HS86, PJH05]. **Triplet** [GV09, GL68, RLF17]. **Triply** [SBDD03]. **Tropospheric** [AVB08]. **Truncation** [Bun18, SDGW98, Bun23]. **Tumors** [Löw65c]. **Tunneling** [LPDB03, MS03, PLA01, Pol03, FTG22, QSW20, Sak03a]. **Twenty** [Ros97]. **Two** [AR03, BC80, BC00, DE05, FP06, HHK+98, HS05, Hyl64, Kri03, LK13, LR72, MDBM98, OM03, PTBH13, QSG98, RA19, SBC09b, SGK+08, VTM98, WHB+24, YZDM01, ZP17, Bar23, BSL+19, CTC22, LPC24, Rui23]. **Two-Band** [Kri03]. **Two-Body** [FP06]. **Two-Bond** [DE05]. **Two-Center** [ZP17, Rui23]. **Two-Colour** [VTM98]. **Two-Component** [YZDM01, Bar23]. **Two-dimensional** [RA19]. **Two-Electron** [BC80, HS05, Hyl64, LK13, OM03, SGK+08, ZP17]. **Two-Particle** [BC00]. **Type** [AYÖ17, AA15, CB92, DR90, GW01, Hog13g, HPB17, PTBH13, SW98, SKT+08, ALA21, KÖO23, Rui23]. **Types** [KS97b].

U [Miy03]. **UC** [SNM+97]. **UFF** [dLHD10]. **Ultra** [KNM+08, VT24].

Ultra-compact [VT24]. **Ultra-Soft** [KNM+08]. **Ultracold** [ML18]. **Ultrafast** [MCP12]. **Unbounded** [Löw88b, LFM89]. **Uncoupling** [MÅ01]. **underlying** [JJ20]. **Unified** [LR72, LJKH13, SO19c]. **Unique** [Ber03]. **Unit** [NA04]. **Unitary** [CDP82, LHL18, Mat78]. **Units** [Moh08]. **Univariate** [Lev14]. **Unrestricted** [BR65]. **Unstable** [ALND10, KG12, MKN10, NBS10, Nic10, NBS12, PD10]. **Until** [Nor98]. **UO** [MCC03]. **upon** [PGJ07]. **Upper** [Wei72]. **Uranyl** [HBT+00]. **Usage** [SPAS05]. **Use** [FSB+97, GMLSC+10, HM21, McG04, MP89, ALA23]. **Used** [Kla81, MKH+97, Pau13]. **Useful** [VKI97, SH19, Wen21]. **Usefulness** [FP06]. **Using** [AYÖ17, AA05, AA15, BS05a, BC09, CB92, CL00, CTG98, Fuk15, GMB04, HJ99, HL90, ILS08, KGW98, KSY08, KB98, KMR01, KV08, LHL18, MCP12, MM96, Mur08, OE17, PJH05, PB75, QGW01, STZY18, SED+98, SGB16, SW98, SYM+08, Uda00, UMD08, VTM98, dLHD10, AA19, BH24, BB22a, Bis19, CCM+19, GDL14, HDFT24, JMWG19, LPC24, MMM19, SA23b, SKS+19, SYIY03]. **Utilization** [ODE75, GG20]. **UV** [BS98]. **UV/VUV** [BS98].

V [TMM03, YIYM03]. **vacancies** [EOH03, Sak03a]. **Vacancy** [NM00]. **Vacuum** [Gre98, Gre08]. **Valence** [CCSZ01, Cse97, FVB99, GVCN82, SH95, SIY+19, WD70]. **Valence-Bond** [GVCN82]. **Valency** [San92]. **Validation** [DSW04, MG21]. **Validity** [Per17]. **Values** [AHPD+03, BKC68]. **Vanadium** [YKC+08, YIYM03]. **Variable** [SGB16]. **Variation** [BLC23, Kar08]. **Variational** [ADRAB16, CTG98, EG99, IM80, LFM89, MM99, MCA+18, OW08, Öhr17, TAU17, WT99, SYIY03, VT24]. **variational-X** [SYIY03]. **Variationally** [GW01, MRHdCK15]. **Various** [JJD05, Kar08, KB86]. **VB** [CTG98, RFG+98]. **Vectors** [GDL14, IM80, Sri01]. **veil** [FSP23]. **Verifying** [BWVD+13]. **Version** [LLBK+98]. **versions** [LH20]. **Vertical** [MLPD+98]. **Very** [Sim07]. **via** [BWVD+13, Gre08, ML18, MCM14, OPPZ06, ÖÖ13, ÖEO23, SIY+19]. **Vibration** [YTC+05]. **Vibrational** [BR17, ILS08, JJD05, Les75, PSAP10, SJO05, SSV98, Tak19]. **Vibronic** [AR03, BP82, Bor03, Chi03, CH03, CHSC03, HDB03, KH03, Kri03, SBC+03]. **Vibronic-induced** [HDB03]. **Vicinal** [SPAS05]. **Vicinity** [MYM08]. **View** [Löw65c]. **VII** [QGW01]. **vinyl** [GC01]. **Violation** [Kar08, QSW20]. **Virial** [LDB95]. **Visualization** [CCVB94]. **vivo** [BB17]. **Volatile** [GAI08]. **Volum** [Ano98f]. **Volume** [Ano64b, Ano65b, Ano67c, Ano68c, Ano70c, Ano72c, Ano73c, Ano77b, Ano80b, Ano81c, Ano81d, Ano82e, Ano85c, Ano98g, Ano98b, Ano98h, Ano98c, Ano98i, Ano01g, Ano01b, Ano01f, Ano08n, Ano09j, Ano10g, Ano10h, SBK04, Ano01d, Ano01a, Ano01e, Ano01h, Ano01c, LSZ+99a, SB17a, SB17b]. **Volumes** [Ano67b, Ano68b, Ano70b, Ano72b, Ano73b, Ano74a, Ano75a, Ano77a, Ano78a, Ano80a, Ano81a, Ano81b, Ano82a, Ano82b, Ano85a]. **vs** [BFHS23, MS03]. **VUV** [BS98].

Waals [LR72]. **wagging** [MFMCN01]. **Was** [Miy03, SEL01]. **Water** [BRL13, CTSDÖ05, CCCC15, CHR13, FCC04, GP14, KBH23, KMHL13, KN01, KV08, RFG+98, RGFC13, SOS13, SIY+15, SCTH+07, SKK23, YMI+21]. **Wave** [BRL13, Bis67, CTG98, Dau64, DB01, FP06, GM17, Har17, Har18, HL97, Joh73, KNN17, LK13, MDÖ05, MS65, Mon05, PSS98, RGFC13, RMMP17, SAL10, Bel22, VT24, SED+98, Sla64]. **Wavefunctions** [HS05, HA13, Sal74, GWW19]. **Wavelengths** [Khe19]. **Wavepackets** [ILS08]. **Way** [PB14]. **Weakly** [KT98, MHWvdA97]. **Weizsäcker** [Cru09c]. **Well** [BRW08, MFCT15]. **wetting** [SYIY03]. **WF** [MKK+01]. **Which** [BR65, GVFR98]. **Wigner** [HW01, HMW01, MH98]. **Wires** [KD11]. **Within** [JGCRC16, Lau09, LJKH13, GWW19, Gut97, SKGŚ23, TM21]. **without** [Ber02]. **WKB** [Pol03]. **WO** [HSS+04]. **Wolniewicz** [PMK23]. **Work** [FU00, KKK+97, SB02]. **Workshop** [Ano98t, Ano98u, Ano01m, Ano01n]. **World** [Ros98]. **Worst** [PS05b].

X [Ada97b, BJMB14, FSB+97, Fuk03, Gut97, IFAY08, Kaw97, KNM+08, MW08, Mur08, NHYU03, OTA97, Ros97, SBA+03, UMD08, YFK+97, Ada00, AAM04, BMC97, CL00, CS77, GM17, HOI+08, Kaw97, KsKsN08, KNM+08, LSZ+00, MYW00, MW08, MKK+00, MTA97, MTA00, Mur03, Mur08, Nak00, SBK+08, SNMI00, SYIY03, Tak19, Tan00, Uda00, UMD08, YKS+12, YFK+97, YNNU03]. **X-Ray** [Ada00, CS77, GM17, Kaw97, KsKsN08, KNM+08, MYW00, MW08, MKK+00, MTA97, MTA00, Mur08, Tak19, Uda00, UMD08, YFK+97, Mur03, YKS+12, YNNU03]. **X-Rays** [AAM04]. **XANES** [KNM+08, MST+03, NM00, YKY+00]. **XHY** [DE05]. **XY** [YTC+05].

years [Cra99, Ros97]. **yl** [NeMM03]. **Yngve** [Lin99, LSZ+99b]. **Young** [Sal74].

Zerner [Sab00]. **Zero** [Dru78, FH65, HBKS03, MYM08]. **Zero-Phonon** [HBKS03]. **Zero-Range** [Dru78]. **Zinc** [MYM08]. **Zn** [FU00, NHYU03]. **Zn-tetraphenylporphyrins** [NHYU03]. **ZnI** [BKC68]. **ZnO** [KNI+08, OTA03]. **Zr** [SMAS08, TMM03].

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