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Title word cross-reference

10 [FK91]. 12 [FK91]. $\textbf{120.00}$ [Gol92]. $\textbf{142.00}$ [Dun90]. $\textbf{152}$ [Dav97].  
1 $\rightarrow$ 4 [GZL94]. 2 [KMM99, SCMV97]. 3 [AT93]. $\textbf{34.95}$ [Gar90]. $\textbf{35.00}$  
[Mez91]. 4 [JFR92a, JFR92b, KMM99, KHG96, SCMV97]. 4 $\leq n \leq 8$ [KT91].  
5 [KHG96]. $\textbf{55.00}$ [Var92]. 6 [FK91, KMM99, SCMV97]. $\textbf{65.00}$ [Klo92].  
$\textbf{72.00}$ [Ran92]. [n] [BRLD92]. + [Cha92, CLS97, GCG97,  
GLLOB91, JKS93, Lôp95b, LDMS99, Mar98, PFFF97, PGBM97, Sie96]. $\dag$  
[GWHD99, GLLOB91, Gre95, GSK95, GG96, Mar98, TRG99]. 2− [SHM99]. 3  
[CGBC96, CLS97, GdAG98, TK94]. α [HMC91, Kik96, Kik99]. $\cdot$, 2+  
[GCG97]. 1 [AVC93, AVP93, CGBC96, GdAG98, MR93, MRG97]. 10  
[MFG91]. 12 [FM99]. 14 [AT93]. 2  
[AS98a, Arn94, AHLR91, BSvRS95, BADP92, BVH92, BSN99, BSS96, \ldots]
/empirical [YM98].

0-947143-84-5 [Ran92].


4-22SP [MHB97]. 4-amino-4-oxo-2-butenoi [Kat90a]. 4-bis [WJL+96, WJV+96]. 4-dihydro-1 [FLHP97, FLPH98]. 4-dihydro-1a [CLQSS98]. 4-dihydropyridines [BHk+91]. 4-dimethoxyphenyl [WJL+96]. 4-dimethylcycloheptane [LCA94]. 4-dioxene [FLHP97].
4-dioxin [FLHP97]. 4-dithiin [FLPH98]. 4-fluorophenyl [Fro93].
4-monosubstituted [SK91, VFM+90]. 4-substituted [AHLR+91].

5 [AT93]. 5-cyclooctadiene [RD97]. 5-Dimethoxy-1 [WJL+96].
5-distyrylpyrazine [ENHE98]. 5-HT [AT93]. 5-tri-[OC98].
5-trimethoxyphenyl [WJV+96]. 5.1 [GPPS91]. 5.21 [GPPS91]. 500-ps [SYHW99].

6 [OJL93]. 6-31G*-based [OJL93]. 6-31g*-derived [CNOJ93].
6-dihydro-1 [FLHP97, FLPH98, PFLH93].

7 [Zho97]. 7-tetrahydroazepines [AVC93].

9-deazaguanine [KG99]. 987X [Ano15].
= [AS98a, BSvRS95, BT92, FBT92, GS90d, JFR92b, Lóp95b, SHM99, SM91, ZY96].

acidities [Kas90, WCK96]. acidity [KH90, KF94, LS96].
acids [ASM+92, BB98a, BKK+96, CBIT94, GKR90, KHF90, Kat90a, Kik99, NTK96, NS98, PC93, Smi99]. across [CA95]. acrylamide [BB96a]. acryloyl [BAPD92]. actinide [SHM99]. action [MSS95, SSM96]. activation [CY98, Vya97]. active [CT97, CG96, FA99, GBE92, HK90, SW+90, SBS99].
active-site [CG96]. activity [AT93, KF94, RdBN90, Ric91].
acyclic
MFG91, OL90, RC93, SUG92, SMF91, VFM+90, WF94, Wel90].

SS93, WMM+95, ACD99, AKF93, BMW+90, BMD99, Ber97b, BRH90, CPR90, DH95, EKS97, FR90, FW92, FS95, GGP96, HB91, KT93b, LPD90, LFB96, MK97a, NVK+97, Pl94, SHM99, VWGF95, AW90, BBH99, CFK97, CT99, CBR99, CG94, GVH94, GP94, GK90, GW95, HY96, JCV+93, Kik96, KJ97, KJ99, LKL+99, MN95, PNJS93, PKN+95, Pet95, RGK93, RTSM93, SM97, TEv90, VBRE93, YTRB97, ZS99, ZM90.

Applications
[Nil91, TKSM96, VVSV96, WCM991, ATK94, BDKJL95, DZSB94, GBW98, JM90, Kio92, SJ95, YTT97, AJ99b, BK79a, FRZ93, HK90, LL98, PS92, WlkJ92, WS93].

applied
[BMN99, DKL90, FPL95, GH98, JM90, Klo92, SJ95, YTT97, AJ99b, BK97a, FRZ93, HK90, LLD98, PS92, WlkJ92, WS93].

Approach
[CN98, AD90, BBR96, BDH+94, BCG97, BFST93, BWS+95, BP93b, Czm98, CC91a, CE96, CS96, DF96, DF97, DM91, DH99, ES99, Flo92, FW93a, GGK98, Gr90, HO93, HY96, JTP93, JA96, Jur96, KW91b, KPi95, LL94, Lin97, ORK+91, PS97, PP98, RM91, RCAA99, SB99b, SBK97, SC95, SM99, SS99, TLBP99, TP93, TS99a, WP97, YM98, YH93, ZY95b, Zho93, ZL94, ZRK+95].

Approaches
[WH95, ALO94, BT96, BM97, BK90, BS96, CKP96, ELA+95, GT96, MRM97, NV91, FM91].

Approaching
[NBB+99].

Approximate
[KKJ97, WSS99a, dVM91, AB90b, ABB99b, AG91, WSS99b, ZG92, ML92].

approximately
[ZS99].

approximation
[ACD97, FRS92, FTA91, AB90b, PS91, PS92, PT99, RH90, RKK90, Tru91].

approximations
[BBS96, AJ99a].

AQUARIUS2
[PMR93].

aqueous
[CG93, CT92, CG94, CG97, CG99, Gao97, GK93, Mar90, NS94, PP93b, Pra93, UF93].

arbitrarily
[TG98].

arbitrary
[JCV+93, Ph90, TAC98, Vya97, YH93].

architecture
[BE98].

area
[BG96a, BG96b, ELA+95, GO95, Her97, LM93, NS94, STPA91, VB93, WL91a].

areas
[FB98, Her93, PC9+92, NS95, WWSS98b, WSS99c, WWSS98a].

argon
[NQ99, Pu97].

ARGOS
[SM90].

aromatic
[BCE+92, DL+97, NPL97, PN93, PMH97, SG92, Sm94].

aromaticity
[FM99].

aromatics
[PS97].

Artificial
[TYRD92, CS94, FPL95, LPD90].

aryl
[FHT99, KHP91].

ASC
[CT95].

ascent
[HKK91].

ascorbic
[ALPH91].

aspects
[CG90, DBS96, Pet94, SN99].

aspirin
[PR9+99].

assemblies
[ELA+95, Te90].

Assessing
[VHK98, VHD+98].

Assessment
[VRBE93, AS97, CSG96, OM96, BG96a, SW96a].

assignment
[BGBW97, CCN90, ORK+91].

assisted
[LL94, VP92].

association
[RTSM93].

asymmetric
[GML94].

Asymmetrization
[GC98].

Asymmetry
[MS98].

atmosphere
[AIDAV98].

atmospheric
[CRSAIVB99].

Atom
[KVL91, BW90, BR97, DFTRJ97, DK97, GKR93, HREK98, LK91, ORK+91, SK93, SB99a, ST94, ZA94, ZKA94].

atom-centered
[BW90, DK97].

atom-type
[ORK+91].

Atomic
[BMK90, DM94, Din91a, DJ92, GM99, Pac95, SH98, WF94, ACD97, AG91, BSS90, BRC94, BCG97, CDR+95, CDG+99, CTS98, Din91b, DH95, DJ93, FR94b, FS94, FCC96].
GPF97, GP94, Kik96, Kik99, KOH97, KE95, LP99, Mar97a, Mar98, ML91, 
Mer92, MHB97, Mul91, NM97, Pac93, PG98, PNJS93, PKN+95, PP97, RL99, 
RC95, SBB+93, SR98, SSRO92, SKOR93, SRI92, SC95, SKM94, Su93, 
TK92, WSS99a, WLKJ92, WR93, Wi94, WFR99, WKP+90, MPJ98.

d atoms [AMY98, BPC91, BC90, CW91, CSC96, DMV98, FB97, GPF97, 
HBLL98, HOL99, IRRR93, JDD97, JLN98, LPT97, LKLB+99, MAP97, 
MH97, PG98, WSS99b, diVM91]. attractive [BPC91].

Automated [LP90, MK97a, MSK92, MGH98, NL98, TAC98, EK97, KW91b, KF94].

Automatic [FSBMP99, BP93b, CCN90, CS94, CF97a]. auxiliary [YG92b].

available [ABD98, GBE92, Hal99b, TJP96]. average [Kik96, Kik99].

Averaged [Mez98, SAdV97]. avoidable [GPF97]. avoiding [BW96].

axial [CPJ98]. axial/equatorial [CPJ98]. azabicyclo


calculates [AFK+95]. Calculating [DM90, ZYY95a, ATS90, CR95, HVM99, KPR91, Mu91, Net94, PZBM98, Pur98, RC95, SKT94, SNS95, VDF+97, WL91a, WO97]. Calculation [Åqv96, BF96, BB98b, DZ97, ER95, GH97, Her93, KOH97, KOH98, KKE93, KSD90, Mit98a, Phi90, RE99, SQ95, SACKH95, ADG99, AC94, ACRC97, BSS90, BG96a, BG96b, CP98, CM92, CG96, CD97, CBR99, Cul92, DKBS97, EA93, Fag91, FW92, FW93a, FB98, FS97, GJR91, GP97, HGC+95, HG93, HW97, KW91b, Kul90, LV90, LD92a, Mar98, MVS92, MSc94, Me92, Mit94, NIS98, NL91, Pet94, RK97, RCAA99, SW96a, SOL97, SMF91, SC95, SKM94, TK99, VS97, WHHP97, WW95, YG92a, vDvdR92, MLA+99].
calculations [MPJ98, MPJC98, MTR90, NCA96, NLA96, NA96, NAA+97, OS98, OBL95, PLY98, Pea94, PR95, PC94a, PFL93, PK91, PN95, RG99, RC93, RP98, RCv96, RCvRS97b, RCvRS97a, RV98, RO96, RLA+98, RHHK90, RSK92, SN90, SD90, SJDW90, SHM99, SKA93, SS93, SN99, SLH96, SKT93, SR94b, SS95, SRI92, SCR93, SCMV97, TP93, TAA94, TNS97a, UF93, VR99, VA94, VSV96, Van99, VW96, VFK92, VW91, VES+99, VA98, VH90, WM95, WZG+93, WF94, WP96, WSS99c, WH95, WJL+96, Wn92, ZA94, ZKA94, ZL94, ZM99, DB91].
calix [VW96]. cam}
[DvRSH94]. **CNDO** [BMD99]. **CNDO/S** [BMD99]. **CO**
[VH99, Dav97, GBT97, BJ94, MRW91, Cha92]. coarse [LMFA92].
**coarse-grain** [LMFA92]. cobalt [UVRCR92]. cobra [SYHW99]. cocaine
[Fro93, VL90, WN91]. code [Ear90, LWNS95, MKF+97, RBC+98]. codes
[DVJ+95a, DVJ+95b, VF98, IG94]. coefficient [KW91b]. coefficients
[BH91b, Gen99, MN92]. Collective [GPB+97, TS99a]. Collective-variable
[GPB+97]. collision [BB96b]. collisional [LB96]. COLUMBUS [DLS+97].
**column** [BR97]. combination [DS90, DRP98, HH99b, KV93].
**combinations** [Flo92, WSS99a]. Combinatorial [TSZ90, GM98b].
Combined [BMW+90, LS94, Rau96, YM98, BT96, BvGMP97, CCJ+99,
CG90, CG98, ER95, FBK90, FG96, FUS+94, PPAS+99, GG96, SR92].
Combining [EKS97, WH93, ZS93, WS99a]. CoMFA [YC95]. Comment
[SC99]. Comments [Bal91a, DHHY90, Ste90, DW98, Hol93]. commonly
[KNST96]. Compact [BC90, HS99]. Comparative
[AGN+90, AVA93, GG96, HL96a, KF99, LIO90, PS98, AT93, Che95b,
EPBD95, FSCS99, KHL96, NVS91, SR94b, YC95]. Comparing
[FPRD99, GW98c]. Comparison [ALO94, AVP93, BP93b, Fag91, FGG+92,
For91, HVS97, HVM99, HK+97, KVK93, KCK98, MSZ96, NBS94, OJL93,
PFFF97, RC95, ST91, SS98b, SW93a, SR98, VVM93, VW91, WR93, WO97,
Wib99, BP93a, Bk93, BC96, BKL+90, DHH90, FGBH90, FRR90,
GWH99, GPP96, GPPS91, GLoNP96, HL96b, JU91, KS96, KHL96,
LHRF93, Lk94, MFG91, MJFT96, MLA+99, RK97, Ric91, RK99, RMS93,
SS93, STB+94, SLH96, Ste90, TS99a, TEHL93, VDF+97, WSV92, WCK96,
AS97, BL91, FW93a, FW98, HVvRS93, HW97, Her97, JB95, JVB95, JLW99,
Kn92, NSA+97, PK95, SUG92, Sul95, TRG99, WM+96, WFW95].
comparisons [FZL97, HO97]. compartmentalization [SOL90].
**Compatibility** [RW99]. complement [SSRO92]. complementarity
[MV91]. complete [WAM91, ZPV+96]. completeness [BKL+90]. complex
[ACD99, Bih99, CFS97, CQSS98, CR95, CG94, DKJ96, KTT94, KTT95,
MGJ99, MP90, NBS93, PDPM97, Yos90, ZS99, ZHBS92]. complexation
[VHWC98]. complexes [Bér97a, BF91, BBS96, CDG+96, CHPK91, CA95,
CY98, FR90, GGK98, GMY97, GSK95, GMO93, Had98, KT93b, KTT94,
KTT95, LHB90, MM93, Mag95, MK+97, MV91, PKCM99, RCAA99,
SCZ99, SH91, SR90, SSO94, TRG99, VW96, VHW98, VHV90, ZY96].
**component** [HBLL98, HNS+97, MPJ98, MPJC98, SRR94, SSR95, SBF91,
TEDV90, VES+99]. components [Gac97, SWOW97]. composed [CDG+99].
**composite** [Bec99a]. composition [BW91a]. compound
[FDMB92, GSB99, PSK98]. compounds
[AF94, An97, BCMZ99, BCF+92, BH98b, BBH99, DDDV93, DDLV95, DVL90,
ER95, FA94, FRC91, FM94, FSCS99, GPPS93, HDA93, JFR92a, JFR92b,
KSP90, LA90, LJ92, LDJ92, LDJ+97, MHI+98, MNVM97, Mar98, MSB95,
MS96, PK95, RdBN90, RR92, Rod94, SHM99, SI93, SW93a, SR94b, SUG92,
TA98, TYMS98, VF92, VW91, WZG+93, WO97]. Comprehensive
[PSY+99, MTRJ95]. compression [FW93b, She90, SCC93]. computational
computations
[ACFO91, FR94b, Gre95, KL91, KV93, RRR92, TRR+94, VS97]. compute
[ALO94, BG93, OL90]. computed [BR97, Fro91, PE92]. Computer
[Bal90, Bal91b, Bal93, LB90, TNKM91, DVJ+, Ear90, El91, HL96b, HEN+, HR97, KW91b, KF94, KUT+, LL94, Mez92, RPG+, SL93, VP92, VHV99]. computer-aided [VHV99]. computer-assisted [LL94, VP92]. computers [BBR96, BDKJL95, CS90, DK93, DPK94, FK95, HA93, LBI+, MD95, MOSD97, MTBS91, RBC+98]. Computing
[ABE+96, ZM90, Dun91, HB91, Ish98a, OS91, ZV96, STPA91]. concentrations [CR95]. concepts [Bic99, PM93, JM90, K192]. concerning
[CHP91, For92, MSZ96, SKT93, YKU96]. configuration
[BBR98, CGBC96, DLS+97, DK90, GBE97, PS96a, RBE98, RSK92, SWK99]. configuration-selecting [SWK99]. configurational
[AGM91, CLO99, WJ+96]. configurations [Kri90, TvG94].
Conformation [CH88, JFFK94, TK94, ATK94, C192, GM90, HO93, HNS+, HMC91, JLW99, KD96, KPR91, MJ93, MM94c, WP97, Dum90].
conformation-dependent [GM90]. Conformational
[AVC93, BCMZ99, BFST93, CT97, CSR92, CC91b, DRF92, Fro93, GJK+, GW95, GK93, HS93a, HP94, HCC99, JJTP93, KS96, KG91, KPI95, KTS92, LMK92, LL98, MNN97, MR93, MRG97, Nic97, PG91, SDD93, SM97, SM91, SW92, SW93b, Su95, SK92b, SOS94, SRS84, TCG96, TJP96, UF93, VGN+, ZLM92, Art93, AW90, BPS93, BP93a, BKL+90, BW90, CHSK96, CEC97, FGG+, FRC91, FPR97, FCS98, GLP95, GSG91, GBE92, GPPS91, GLoNP96, HN96, HNL99b, HHH91, HBR+, IMP91, JLW97, KMK98, KG99, Kuc96, LPD90, LP90, LSR97, LSD99, LCA94, MK98, MK94, MJFT96, MJLV92, NBS94, NIS98, NWAM95, PD92, RP97, RD97, RPR+, ST92, SB98b, STT95, SB99b, SACKH95, Sun94, SCM95, VRC91, VRC92, VTR+, VL90, WMM+95, Wa97, WHF97, WSV92, WCM99].
Conformational [BP93a, BB96a, Cso93, Gho98, KG93, LRS97, PHG94].
conformational-determining [NWAM95]. conformationally
[KVL91, MKS90]. conformations [ALPH91, BK97a, BGZP97, BSV94, Dav93, FM94, GHR93, HC95, KF99, LHB93, Luk94, Mez98, Ob98, PS91, Par99, PMIB99, SSD93, SM94, Snu92, TEHL93, We90, vFB91]. Conformers
[ZCP98, BSC+98, BB95, FLP98, PFC96, PE92, Sau91, SJV93, WMM+95].
congeners [GPK95]. conjugated
[ALYT90, BB96a, KL91, MSB96, NLA96, NA96, TA98]. conjugated-circuit
[KL91]. conjugation [Che95b, CD97, WMM++95]. connection [AB98a].
connectivities [GM98a]. conquer [PLY98, SHCY93]. conrotation
[MQS++97]. Consensus [BBH99]. Consequences [LP99, BvH++92].
conservation [Har93, ZS95]. Conserving [KHW++90]. consideration
[CD97, fGGG94]. considerations [KT93a]. Consistent
[AJ99a, AJ99b, GH98, FRSNS92, FCNSÁ98, FW92, FM91, Gre95, HOL98,
HGK++96, JHB96, MPJ98, MPJC98, RW99, TRR++94, WH95]. constant
[ACRC97, EGH++93, GdAG++98, MGLL99, McD97, YC95, SB99a, SW96b].
Constant-NT [SW96b]. constants
[BP98, BPC91, CgdAC91, Dum91, DBT98, FM99, GKM94, GH97,
KHF90, KHF91, KKH91, MFG91, PPK92, Phi90, Pol93, RCAA99, WL91b].
Constrained [BB93, Bak97, BKLS95, Bla91, DRRK95, FSW96, Bak92].
Constraint [WS98, FS98a, FS00, GK90, HBBF97]. constraints
[KID93, LZT91, PHG94]. Construction
[CHP90, PPK91, FTW++96, RWB99]. containing
[BCB++97, BB98a, CW91, DJ94, HBL98, HDA93, IS91, LA90, Mar98,
MS95, MSB96, PKN++95, SAF93, SE95]. Continuous
[KRL++93, SA99, CBR97]. continuum
[BCT98, BF96, CTP95, CMPT98, FTA91, GMM95, HY96, MRS98, PT98,
PTCB99, PKCM99, PN95, RCB99, SC99, TRLRB96, WS99a, Zau91, dVA92].
contouring [ELA++95]. contracted [BC90, DKH98]. contribution
controlled [SHH90]. controlling [BSC++98]. conventional [AB98a].
convergence [AL98, BBR98, DM91, DBS96, MM93, Pea94]. convergent
[GS94c, She90]. conversions [BRLD92]. cooled [Su95]. cooperativity
[KLC++98]. coordinate [Bec98, FZL97, GLP95, Ish98a, JDD97, JLN98,
KG91, Kg93, Maz97, Pol93, TA94]. coordinated [BBC++98]. coordinates
[AC94, BH91a, Bak92, BB93, Bak93, BC96, Bak97, Bec97, Bør97a, BSS++97,
CMC96, LPP99, ML91, MKS97, NIS98, PPK92, PAS96, PP98, RS92, SG95].
Coordination [Mar90, GS90d]. Copenhagen [Tay99]. copper [CG93]. core
[Cso93, Ear93, GC97, HHC90, KS97, LL92, RCATD96, SR94b].
core-repulsion [Cso93]. corrected [HVM99, KK91]. Correction
[CMPT98, CFK97, DW98, GW91, PS98, SKOR93, TEdV90, VVM93].
corrections [Aro97, Bec99b, FV98, Klo97, Kut99]. Correlated
[Gen99, RSK92, VRV99, KA92, KK91, PL94, SKA93, SLH96, WLC92,
ZA94, ZKA94]. correlating [KNST96]. Correlation
[KHF90, KHF91, dVA92, BPP90, BP93b, BS99, CB96, DH90a, FR94b,
Gen99, GCG97, HKY98, HHC90, ISH98b, Klo97, MAP97, MPJ98, MPJC98,
RW99, SI93, SS97, SB92a, SBS99, TA98, Zho93, ZL94, BW91a, SYHW99].
correlation-consistent [RW99]. corresponding [BMN95, Mit94]. coexistent
[RR92]. Coulomb [ADG99, KHL96]. Coulombic [LLD98, SKT93].
Counterpoise [KK91, TEdV90, TEdV91]. counting [BK97b]. Coupled
[CG97, CG99, FKN⁺93, Kar99, MRS98, RGK93, SHM95, TMCM⁺96].
coupled-cluster [RGK93]. coupling [BBR98, BSN99, CGdAC91, EGH⁺93,
GdAG⁺98, RCAA99, TEdV90, VES⁺99]. couplings [O’m99, VRV99].
covalent [ER95, WB91]. CP [TEdV90]. Cray [SOCF98]. Crick [SCZC99].
Crippen [Dun90]. criterion [RWB99]. criterion [RBC⁺98, Yos90]. Critical
[CEA92, EK97, SSV93, DV99, FB97, Gri90, HD92, MvRSL⁺97, MFG91,
TEHL93]. critical-point [FB97]. crossing [AB97, FD91]. crown
[LHBF93, SK92b]. crown6 [VW96]. cryptand [AW90]. cryptophane
PKCM99, VHW98]. Crystal
[MvEP⁺98, YTT97, HDA93, KG92, KRL⁺93, KRM92, LOP⁺97, PRRD98,
VK97, VTR⁺94, WS93, WPLC95, WJL⁺96, vEK99]. crystalline
[DDV93, DVL90, EKS97, HYH⁺94, TM95, Dil95b]. crystallography
[BSL91, SYHW99]. crystals
[ACRC97, FCNSÅ8, KVKK93, LYH⁺95, SWAH91]. Cs [JLN98]. Csonka
[Ano15]. Cu [SW⁺90, SMA92, TKSM96]. cube [HTC98, HGB93]. cubic
[ACRC97, ELA⁺95]. Cumulative [Pet93, SRO92]. curves
[BG93, PLB92, WB91]. cutoff [GZ95, SB94]. CVFF [HKŠ⁺97]. cyanates
[LS98]. cyanoketene [CLQSS98]. cyclic [Che95b, CD97]. HVvRS93, KG93,
KHG96, MV91, NBB⁺99, PD92, PHG94, TA98]. cyclization [LK90].
cycloaddition [ARLG⁺94, NVER97, SSQ92]. cycloadditions
[CN98, MP98]. cycloalkanes [Cri92, WA99]. cycloalkene [SJV93].
cycloextrin [BPZL96, WSV92]. cyclohexaglycine [BB95].
cyclohexanetriol [BPZL96]. cyclooctadiene [RD97]. cyclooctane
[RPR⁺98]. cyclopentadieny1 [RvRS98]. cyclopentane [CHSK96, Jai90].
cyclopentenes [Bal98]. cyclopropeniumyldiazonium [Gla90].
cyclochrome [BO93, HL96a, Kat93]. cytosine [RTGJ98, SLH96].
D [AT93, AVC93, AVP93, BO93, Ear90, GH98, MNVM97, MK94, NL91,
SHCY93]. D-CICADA [MK94]. D-norcamphor [BO93]. data
[Als95, BG93, BB98a, FSW96, FM94, GSB99, Hal96d, HGB93, HBR⁺99,
KFM99, LHBF93, LOP⁺97, MTH94, MM97, Mer92, MLA⁺99, NL98,
PGAL93, RGK93, SAdV97, Sh90, SC95, SYHW99, VTR⁺94, WAW⁺97,
YB94, YB95b]. database [EK97, MK97a, AGN⁺90, LHBF93]. databases
[Fel96]. David [Dav97]. Davidson [Cl93, VSV96, vLP90]. Davydov
[För92]. DD [BSL91]. DD-peptidase [BSL91]. DDRP [DBS93]. dead
[GM98b]. dead-end [GM98b]. deaminase [HK90]. deazaguanine [KG99].
dea zapterin [CG96]. debate [Ove91]. deca [KG91]. deca-alanine [KG91].
decahydroisoquinoline [MR93]. decarboxylation [NBG93]. decaying
[LP99]. Decomposition
[KT94, KTT95, ABBC99b, BBR96, DH90b, LZZ98, WAW⁺97, YB94].
Decoupling [BBS96]. dediazoni ation [Gla90]. dedicated [CGBC96].
deduced [Pae95]. deduction [Cri95]. defined [DBS96]. defining [PP98].
DefPol [PT98, PTCB99]. degenerate [Ber97b, GML94]. degradable
[PC94b]. degradation [PC93]. degrees [Bér97a, DMB91, SEJ95].
dehydroamino [AGP91]. dehydrogenase [vOC93]. delocalized
[Bak97, RCv96, RCvRS97b]. Demonstrations [DPK94]. Dennis [Ran92].
dense [CRME93, CB96]. densities [LP99, Mez98, O’m99, WAM91].
Density [CAC99, HsR95, Jur96, RJP97, SHM99, VKC96, AB98a, ACD97,
ACD99, Ano15, AGM91, Bec99b, Ber97b, BKMH97, BW90, Che99, CRP97,
CH96b, CEC97, CNK97, ED99, ES99, For96, FV98, GWHD99, Gla90,
GPF97, GHT98, GW91, HGC+95, HK95, JH98, KS96, KA96a, KE95, Koh99,
KCK98, LSC98, LDG99, LMB96, LWNS95, LP99, LBA+99, LKL+99,
MrVSL+97, MSDC94, MRS98, MN92, MPJ98, MPJC98, MTR90, NVA+97,
NVK+97, O’m99, Pac93, Pac95, PSY+99, PK95, Rau96, RTGJ98, SLPP97,
SBA97, STB+94, SLH96, SOL97, SACKH95, SHM95, SVS+97, TMCM+96,
Van97, Van99, VA98, VSF97, Wib99, ZG92]. density-dependent [Pac93].
deoxythymidine [ST92]. dependence [HK95, JH98, MN92, SBA97, SB92a, SW92, SW93b, UF93, RE99].
dependency [GKM94]. dependent [BBvG95, DH95, GM90, KVL91, KD91, MKS90, Pac93, RNDP98]. depleted
[LBA+99]. Derivation [DA96, GDK92, MH+94, MJH+98, WK+90, CCB95, Hil97, Su93, Din91b].
derivative [BB96a, JK98, Mil90, SMS98, SFB91, TA94, AS98b].
Derivative-free [AS98b]. derivatives [AYC94, AS98b, AHLR+91, BPZL96,
BK96, CW91, CM96, DH90b, GS90a, Hi98, HM91, HW+91, KHB92,
KB92, KPR91, LKL+97, LBB94, LFB96, MOS97, McD96, NS98, PT96,
Pea94, PCG+92, SK92a, SNS95, SB92b, VTR+94]. derived
[AL093, BC93, BCG97, BMK90, CNOJ93, CK91, DMB91, DW98, FRR90,
Fer91, HE99a, Kik96, Kik99, Mar97a, Mar98, Mer92, PS91, PS92, RC95,
SSD93, Spa96, SBS99, SW92, SW93b, UF93, WF94, WR93]. deriving
[S98]. describing [HS99, MLAT99, MLA+99, SOL90]. description
[BMD99, EBD+99, GLP95, GGP96, JB98, KE95, LDG99, PSS98, P98,
PaST94, Si96, STPA91]. descriptions [MM94a]. Descriptors
[NS98, BR97, KHL96, SK92]. Design [CR90, LJKL98, SLPP97, Tay99,
AT94, AFK+95, CS94, DLK90, LL94, TMK+99]. desulfuration [Kat93].
detailed [AB+96]. Detection [AW91, WSS99b]. Determination
[FSW96, ML91, PNJ89, PKN+95, YSJ95, EG+93, FD91, Gen99, LPW+97,
MLB92, MJ93, NKA98, PCG+92, YB95]. determined
[PK98, WWXS97, Zau91]. Determining [BW90, NWAM95, SR90].
deterministic [KFML99]. deuterium [EG+93]. developed
[DHRY90, Ste90]. Development [HS95b].
Diabatic [KCK97, PLB92]. diacetate [Fag91]. diagonal [CHSK96]. diagrams [KRL+93]. diamines [LSDB99].
diaminobenzene [KTT94, KTT95]. diaminodichloroplatinum [ACD99].
Dispersion [FTA91, LLB99]. Display [SR94a]. disrotation [MQS97].
dissociation [Kri90]. dissociative [PLB92]. dissolved [DS92]. Distance
[CH88, Bal90, GHR93, GHR94, JCV93, PD92, Pet95, WSV92, PP97, Dun90].
distances [Kik96, Kik99]. distinct [GSB99].
distortion [ATK94].
distributed-memory [CS90, DK93, LMCPP92, CS96].
distances [CH88, Bal90, GHR93, GHR94, JCV93, PD92, Pet95, WSV92, PP97, Dun90].
distances [Kik96, Kik99]. distinct [GSB99].
distortion [ATK94].
distributed-memory [CS90, DK93, LMCPP92, CS96].
distances [CH88, Bal90, GHR93, GHR94, JCV93, PD92, Pet95, WSV92, PP97, Dun90].
distances [Kik96, Kik99]. distinct [GSB99].
distortion [ATK94].
Distributed [RGK93, BDKJL95, CS90, DK93, Fer91, FK95, Lim97, LMCPP92, MD95, MOSD97, PFM91, WPLC95, CS96].
distances [Kik96, Kik99]. distinct [GSB99].
distortion [ATK94].
Distributed [RGK93, BDKJL95, CS90, DK93, Fer91, FK95, Lim97, LMCPP92, MD95, MOSD97, PFM91, WPLC95, CS96].

eigenvalues [BB98b, CMC92, Mit94]. eigenvector [KV93, vLP90]. eigenvectors [CMC92, Mit94]. ELECT [MK98]. Electric [HMS93, CEÅ92, GSW90, McD97, Wil94, ZM90, ZYY95a]. electrolyte [YL90]. Electron [BSN99, FSCS99, LTHY96, LH99, PD99, AGM91, AD90, BPP90, CW97, CC98, Cu92, FPC91, FW93b, Gla90, GCG97, GL99, HKY98, IS91, JU91, KJ97, LO98, MRH99, MRS98, PSK98, PMIB99, PC94b, Sadv97, Si93, SMA92, SSV93, SH98, SMF91, SKK+93, TRG99, VB93, WCK96, YL90, ZV96, dVA92, SS97, WZG+93]. Efficiency [BM99, MM97, BKL+90, CW93, EA93, ET98, FHB99, OM96, SS93]. Efficient [ADG99, CSC96, CBSR99, GLP95, GM90, RS92, SKT93, TA94, TN97a, Wan97, vFB91, AS96, BM99, CBSB94, FB98, GS94b, HS95b, KO97, KV93, NIS98, PS97, SC95, SJ95, ZV96, ELA+95, FCS98, FS98a, FS00, KMKW97, WH99].

eigenvalues [BB98b, CMC92, Mit94]. eigenvector [KV93, vLP90]. eigenvectors [CMC92, Mit94]. ELECT [MK98]. Electric [HMS93, CEÅ92, GSW90, McD97, Wil94, ZM90, ZYY95a]. electrolyte [YL90]. Electron [BSN99, FSCS99, LTHY96, LH99, PD99, AGM91, AD90, BPP90, CW97, CC98, Cu92, FPC91, FW93b, Gla90, GCG97, GL99, HKY98, IS91, JU91, KJ97, LO98, MRH99, MRS98, PSK98, PMIB99, PC94b, Sadv97, Si93, SMA92, SSV93, SH98, SMF91, SKK+93, TRG99, VB93, WCK96, YL90, ZV96, dVA92, SS97, WZG+93]. Efficiency [BM99, MM97, BKL+90, CW93, EA93, ET98, FHB99, OM96, SS93]. Efficient [ADG99, CSC96, CBSR99, GLP95, GM90, RS92, SKT93, TA94, TN97a, Wan97, vFB91, AS96, BM99, CBSB94, FB98, GS94b, HS95b, KO97, KV93, NIS98, PS97, SC95, SJ95, ZV96, ELA+95, FCS98, FS98a, FS00, KMKW97, WH99].

eigenvalues [BB98b, CMC92, Mit94]. eigenvector [KV93, vLP90]. eigenvectors [CMC92, Mit94]. ELECT [MK98]. Electric [HMS93, CEÅ92, GSW90, McD97, Wil94, ZM90, ZYY95a]. electrolyte [YL90]. Electron [BSN99, FSCS99, LTHY96, LH99, PD99, AGM91, AD90, BPP90, CW97, CC98, Cu92, FPC91, FW93b, Gla90, GCG97, GL99, HKY98, IS91, JU91, KJ97, LO98, MRH99, MRS98, PSK98, PMIB99, PC94b, Sadv97, Si93, SMA92, SSV93, SH98, SMF91, SKK+93, TRG99, VB93, WCK96, YL90, ZV96, dVA92, SS97, WZG+93]. Efficiency [BM99, MM97, BKL+90, CW93, EA93, ET98, FHB99, OM96, SS93]. Efficient [ADG99, CSC96, CBSR99, GLP95, GM90, RS92, SKT93, TA94, TN97a, Wan97, vFB91, AS96, BM99, CBSB94, FB98, GS94b, HS95b, KO97, KV93, NIS98, PS97, SC95, SJ95, ZV96, ELA+95, FCS98, FS98a, FS00, KMKW97, WH99].

eigenvalues [BB98b, CMC92, Mit94]. eigenvector [KV93, vLP90]. eigenvectors [CMC92, Mit94]. ELECT [MK98]. Electric [HMS93, CEÅ92, GSW90, McD97, Wil94, ZM90, ZYY95a]. electrolyte [YL90]. Electron [BSN99, FSCS99, LTHY96, LH99, PD99, AGM91, AD90, BPP90, CW97, CC98, Cu92, FPC91, FW93b, Gla90, GCG97, GL99, HKY98, IS91, JU91, KJ97, LO98, MRH99, MRS98, PSK98, PMIB99, PC94b, Sadv97, Si93, SMA92, SSV93, SH98, SMF91, SKK+93, TRG99, VB93, WCK96, YL90, ZV96, dVA92, AB90, NVK+97]. electron-repulsion [Jon91].

Electronegativity [HD92, PN93, PKN+95]. Electronic [Dav97, MTR90, RdBN90, ACD99, BA94, BCFM98, Bog99, BR97, Cai94, CBWF98, CI93, DKJ96, FR93, LWN95, Lód95a, Lód95b, MV97, MM93, MKF+97, PZBM98, SV94, SD90, SBB+93, SC91, TAC98, UVR92, WAM93, We90, WLC92, Yar95, ZM99]. electrons [SWOW97].

Electrostatic [BF91, FR93, LDM92a, Mag95, PK98, PSW96, SW96a, Áqv96, AG90, ALO93, ALO94, AVA93, AHI+91, BT96, BRC94, BCC97, BF96, BCF+92, BW00, BNDS97, BBH99, CPR90, CK91, DM90, Din91a, DA96, DP95, DKB97, EGH97, FO93, FW93a, FCG96, GMM95, Hal96b, HE99a, HE99b, KK97, KL96, LCW93, LIO90, Mar97a, Mar97b, Mar98, Mer92, MGPR90, NTK96, Non97, OL90, Pet93, PS96b, PF91, PDF97, RC93, Ric91, RC95, RMS93, SADV97, SWS+90, SKT94, SR98, SSR92, SOL97, SACK95, SW92, SW93b, Su93, SJ95, UF93, VS97, WF94, WLK92, WA99, WPLC95, WK+90, ZV96, Mar97a, Mar97b, WM94].

electrostatically [RPG+95]. electrostatics [RPG+95].

element [BvGMP97, BWS95, CF97a, CF97b, FR94b, FR93, FUS+94, NL91, PN95, Pur98, VS97, WW98, YL90, YH93, ZV96]. elementary [ACD97, VP93].
elements [AJ99b, AC94, IG94, KTK93, LH99, Mil90, SB95, ZL94].
elimination [GM98b, ZP99+96, BK96, GPF97]. ellisoidal [FW92].
elucidated [KG99]. elucidation [MK94, VP92]. elusive [Har99b].
embedded [GHS97, ZY96]. embedding [CSR92, Cri92, IRR93]. emphasis
[WHF97]. Empirical [RC9vRS97b, RC9vRS97a, BFST93, Di90, Di92, Di95a,
Di95b, DW98, EJ95, Hal96d, HG93, HNH+91, HK97+97, MKS90, MGH+98,
NTK96, RK97, RC9v, SLH96, VB93]. empirically [SB90]. employing
[SLPP97]. enamines [AYC94]. enantiomeric [DKL92]. Enantioselective
[BPZL96]. enantioselectivity [Aer95]. end [BH91a, GM98b]. ended
[ABD90, AD90]. endo [CGdAC91, JZ96]. endo-endo [CGdAC91].
elusive [Har99b]. elucidation [KG99]. elucidated [KG99]. ellisoidal
[FW92]. emphasis [WHF97]. Empirical [RC9vRS97b, RC9vRS97a, BFST93, Di90, Di92, Di95a,
Di95b, DW98, EJ95, Hal96d, HG93, HNH+91, HK97+97, MKS90, MGH+98,
NTK96, RK97, RC9v, SLH96, VB93]. empirically [SB90]. employing
[SLPP97]. enamines [AYC94]. enantiomeric [DKL92]. Enantioselective
[BPZL96]. enantioselectivity [Aer95]. end [BH91a, GM98b]. ended
[ABD90, AD90]. endo [CGdAC91, JZ96]. endo-endo [CGdAC91].
elusive [Har99b]. elucidation [KG99]. elucidated [KG99]. ellisoidal
[FW92]. emphasized [GHS97, ZY96]. embedding [CSR92, Cri92, IRR93].
empirically [SB90]. employing [SLPP97]. enamines [AYC94]. enantiomeric
[DKL92]. Enantioselective [BPZL96]. enantioselectivity [Aer95]. end
[BH91a, GM98b]. ended [ABD90, AD90]. endo [CGdAC91, JZ96]. endo-endo
[CGdAC91].
[Mit94, NH91, SOL90, SBA97, SW96a, TG98, ZYY95b, ZPV+96].

**equations**
[KTnH99, LMB96, Maz97, Pol90, Ram90, RPGS97, SBJ92, WS99b].

**equilibria**
[CPJ98, Fab91, NBS94]. **equilibrium**
[CR95, LV90, MM95, PASF96, TRLRB96]. **equipartition**
[HTC98].

**equivalent**
[BR97, SC94, VK97]. **erased**
[BW96]. **Errata**
[KTT95, SSR95].

**Erratum**
[Ano15, FS00, WWSS98a]. **Error**
[AFK+95, IC96, HVM99, WB91, KZ99]. **errors**
[AG90, BG96a, CMPT98, DB98, GPF97, RK97]. **essential**
[VDF+97]. **ester**
[DLM+98, LMB99, LPT97]. **esters**
[ASM+92, FBTD92, GM99]. **estimate**
[AVP93].

**estimated**
[HI98]. **estimates**
[RK97]. **Estimating**
[MAP97, SVM99, NBS94]. **Estimation**
[DJ93, CB96, DNC96, HK92, VTR+94].

**ethane**
[HMG96, MS98].

**ethanediol**
[RBSB96].

**ethanes**
[CPS90].

**ethanol**
[LPT97].

**ethers**
[BMJ90, VRC91, VRC92].

**ethyl**
[EPBD95, FBTD92].

**ethylene**
[BPS93, Fag91, JB98, LV90, MSSS95].

**ethylenes**
[MP98].

**ethylenic**
[JB98].

**ethylnitrene**
[KW91a].

**Evaluating**
[BDKJL95]. **Evaluation**
[GJR91, GHT98, GMO93, ISH98b, JCV+93, LP95, MGPR90, Vya97, AFEO91, AFK+95, ABD90, BBR96, CDR+95, CS95, CTC95, DV99, EGHT97, EK97, Fer95, GP94, HA93, HW97, KW91b, KF94, Lim97, LWS+95, MS92, MJSV92, NTK96, RKL93, TRG99, WCC91, YG92b, ZG92, Ziv+90].

**evaluations**
[OJL93].

**Evans**
[ABB99a, ABBC99b].

**events**
[SB98a].

**evidence**
[LP92].

**evolution**
[LMB96].

**Ewald**
[CÇG97, DKBS97, KVKK93].

**Exact**
[FB98, SW99b, BK97b]. **exactly**
[GS97].

**examination**
[KWWS91, SM95]. **example**
[ACD99, DB98, JZ96, HREK98]. **excess**
[SW96b].

**exchange**
[AB98a, FS98b, GW91, HVvRS93, HREK98, LP99, MQS+97, RCAA99].

**Excitation**
[HT99a, BA94, Gri94, RSK92].

**excited**
[CT98, F99, FRZ93, GWHD99, GJCC93, RSK92, WLKJ92].

**excited-state**
[FA99, GWHD99]. **excluded**
[Bla91, GO5, KPR91].

**excluding**
[PaST94].

**Exhaustive**
[BV97].

**existence**
[SS95].

**Exo**
[CGdAC91].

**Exo-exo**
[CGdAC91].

**expanded**
[TSZ90].

**Expanding**
[LCA94].

**expansion**
[Ish98a, MGPR90, PG98].

**Experiences**
[DBS93].

**experiment**
[JU91, NSA+97, Suf95, WWF95, Obe98]. **experimental**
[Hal96d, Her93, MLA+99, NL98, PK95, SUG92, SF96, Wib99].

**expert**
[CCN90].

**Explicitly**
[ZA94, KA92, SKA93, ZKA94].

**Exploiting**
[MRM97].

**exploratory**
[GS90b, KW91a].

**Exploring**
[Bec99b, Cri92, SM98, JLV97, PFFF97, SBA97].

**exponential**
[CDR+95].

**exponential-type**
[CDR+95].

**exponentially**
[LP99]. **exponents**
[CR95, GvRSvEH+93, Mag93b].

**expression**
[MN92].

**expressions**
[SF92].

**Extended**
[HM90, ML92, BM95, DJ94, EHNW96].

**Extension**
[LDJ92, LBAO96, MKF+97, PS97, WSS99c, Hal96d, Mar98, Ste91].
Extensions [HA95]. extensive [HK95]. external [Yos94]. extraction [VW96]. extrapolation [CW93]. extraribosomal [Dav94b].

**F** [AS98a, BSvRS95, BT92, Dun90, Jur96, SHM99, SI93, SM91, Tay99, DJ94, HDA93, KMM99]. **F-containing** [HDA93]. **Factors** [BSC+98, BSvRS95, BT92, Dun90, Jur96, SHM99, SI93, SM91, Tay99, DJ94, HDA93, KMM99]. **F-containing** [HDA93]. **Factors** [BSC+98, BSvRS95, BT92, Dun90, Jur96, SHM99, SI93, SM91, Tay99, DJ94, HDA93, KMM99].


H [BSvRS95, BKMH97, CLS+97, FM99, GMY97, IBKvRS92, JKS93, KG99, Lóp95b, LSvRS96, MI99, Mez91, Ran92, SM91, TDFdC91, VHV90, ZMC+97, KTS92, AG90, AC94, ACD99, AHL+91, CLQSS98, Che95a, DJ94, DB593, FLHP97, FLP98, GrVSaEH+93, GMY97, GSW90, HDA93, LDMS99, Mag95, MR99, MQS+97, NL91, PT99, RNNDP98, RR92, SBM97, Sie96, TED90, VCLB92, ZMC+97]. H- [HDA93]. -1 [KTS92, FLHP97, FLP98]. H-azirine [CLQSS98]. H-bonded [AG90]. H-chromophores [Che95a]. H-phosphole [SBM97]. H/He [GSW90]. Hadamard [Bal93]. half [OS91]. half-projected [OS91]. halide [LK90].
Interactions [RLG98, Aqv96, BF91, CKP96, DM94, DH90b, DW98, DKBS97, EGHT97, FM91, GK93, Hal96b, Her93, HLS99, HC96, KID93, LDG99, LYH+95, LPW+97, LWS+95, MLAT99, MLA+99, Nil91, Non97, NWÄM95, Ove91, PPAS+99, PDPM97, RK95, SKT93, SKT94, TMB93, TNS97a, TNS97b, YB94, ZM92].

Interactive [CS94], interatomic [HC96], intercalating [SUG92], interconversion [ORK+91, Sau91], interconversions [LCA94], interdiffusion [DF96].

Interested [DDV93, DDLV95, DVL90, Mul91, SACKH95].

Interface [PMIB99, TYMS98, VW96, VM95].

Intermediate [SSQ92].

Intermediates [CLQSS98, ZVP98].

Intermolecular [BMN95, FM91, HVM99, Hal96b, Hal99b, HREK98, KTT94, TMB93, TNS97a, TNS97b, YB94, ZM92].

Intermolecular-interaction [Hal99b].

Internal [EPBD95, FZL97, MQS+97, Yos94, Yos96, Bak93, BC96, Bak97, Bér97a, BADP92, CPS90, FBTD92, GLP95, KG93, LPK99, LM96, MS98, Maz97, NIS98, PPK92, PASF96, Pol93, PP98, SGB91, TDFdC91, TA94, Tru91].

Internally [DKH98].

Internuclear [Mag93a].

Interparticle [YB94].

Interpenetrating [AW91].

Interpolation [BvGMP97].

Interpretation [SHCY93, KLR96].

Interscience [Mez91].

Intersecting [Jen94].

Intervals [Cri95].

Intra [KWWS91].

Intramolecular [BA94, ČTS98, DP95, FA99, HKK+97, KKCH96, LK90, RBSB96, RR92, Rod94, SCHR97, SV93, FVR92, VRC92].

Intrinsic [AT93].

Invariance [AGM91].

Invariants [BC93, DMB91].

Inverse [JCV+93, RPGS97].

Inverse-square [JCV93].

Inversion [CT95, IC96, KTH99, SMS98, SR92].

Investigating [AM99].

Investigation [ZY96, BB96a, BS95, BVH+92, Gre95, GG96, HL96b, JB98, KB92, KPSM98, LZS98, RTGJ98, SBM97, TRG99, WM93].

Investigations [BH98b, RBSB96, SI93].

Involving [BW91b, CG90, FPSK92, HHC90, LKL+97, SR92].

Iodides [CPR90].

Ion [CG90, CG98, GCG97, GMO93, LS98, PBS97, Sha91, TD95].

Ion-neutral [GMO93].

Ionic [PFM97, RM91, SCR93].

Ionization [ABE+96, CC98, GJR91, HG93, ML92].

Iodized [CG99, HMG96].

Iodophores [BMW+90].

Ions [CG94, FHT99, Gla90, JAdV96, Sie96, VFM+90].

IPPP [CGdAC91].

IPPP-CLOPPA [CGdAC91].

IRCC [ZMC+97].

ISBN [Ran92, Tay99].

Isocyanates [LS98].

Isodensity [JK99, WAM93].

Isodesmic [WO97].

Isolated [AOYY96, ARLAB99].

Isomer [GJCC93].

Isomeric [BH91b].

Isomerization [CBS99, Jur96, VCK96].

Isomerizations [Bal98].

Isomers [AOYY96, BS95, BRD92, BVH+92, HMG96, IBKvRS92, RJP97, SCP92, VK94, WIV+96].

Isomorphism [LK91].

Isotope [JU91].

Isotopic [ZVP98].

Iterated [DNC96].

Iteration [RPGS97, VVS96].

Iterative [Mit94, IC96, KTH99, KPV96, She90, SB99b, CT95].

IV [CW97, DDLV95, DMB91, HN96, PKN+95, ZL94, dVA92].

Ix [Mez91].
HBBF97, LDM92b, Mil90, PHG94, Ram90, WSS99a, ZYY95b. linearized
[CSR92, Cri92, SW96a]. linkages [DDLV95, SE94]. linked
[FS98a, FS00, GZ94, ITP90]. linoleoyl [LH96]. lipid
[CCJ+99, HP94, SWAH91, SW92, TM95, WS93]. lipophilicity [VRBE93].
lipopolysaccharide [KM96]. liquid [BMJ90, EGH+93, FB97, GZ95, GDK92, JLNTR93, Mez92, TM95, TMCM+96]. liquid-crystalline [TM95].
liquids [FSBMP99]. list [GBE97, RBC+98, RBE98, WWSS98b, WS98a].
lithium [AKF93]. liver [vOC93]. LMOs [KK91]. load [YB95b]. Local
[LKLB+99, BSS90, BP93b, CN98, CS95, GS90c, GW91, MTR90, RPW98, SB99b, SB90, TRR+94]. local-density [GW91]. Local-scaling [LKLB+99].
local-spin-density [MTR90]. Localization [CS95, FSCS99, KS97].
localizations [BP93b]. Localized
[Cul92, KKE93, RCv96, Zho93, ZL94, BCFM98]. Locally
[Vas92, CRME93, CB96]. locate [AB98b]. locates [Sno92]. locating
[AB97, BG99, BoF94, BC95]. location [BC96, Har99b]. logic [LM93]. logical
[YB94]. lone [JZ96, Pra93]. Long
[BPC91, GJD94, Kna92, Ric93, Åqv96, LOP+97, SB94, TM93, KID93].
Long-range [Ric93, Åqv96, LOP+97, SB94, TM93]. Long-time
[BW96, CE96, DH99, ZRVD93, P91, WS99b]. Loop-erased
[BW96]. loops [DS90, GS97, P92]. loosely [FKN+93]. LORC [FGHB90].
Low-barrier [KPSM98]. low-energy [BB95]. low-level [BBS96]. low-lying
[Cai94]. Low-mode [KG99]. low-order [Har99b, RPW98]. low-pressure
LTB [GW95]. Ltd [Dav97]. LUMO [YC95]. lying [Cai94]. Lysine
[HNH+91]. Lysine-Alanine-Alanine [HNH+91]. lysozyme
[EHNW96, PS92].

M [BT92, Dun90, GD98, JFR92b, Klov92, HK97, JFR92b, KW99, Mar97a, Mar98, SUG92, GD98, JFR92b]. m-AMSA [SUG92]. machines [Lim97].
macroyclic [Wan97]. MACROMODEL [TJP96, MRG+90].
Macromolecular [Ske91, DKRR95, LK92, PH96, SB94, V97, WM95].
macromolecules
[FB98, MTBS91, Pur98, SB99b, WL91a, WS98, Y93, ZKS93, ZYY95a].
Madelung [FCNS99, FMM97, SCR93]. Maggiora [Klov92]. magic
[JKS93]. magnesium [CHPK91, GS93, KSP90]. magnetic
[BG99, CCN90, CRME93, EBD+99, EPBD95, FGH90, FSW96, K99, MV97, MV98]. main [BK97a, ENvRS94, HK95]. maleamic [Kat90a].
Man [Cas99, Gar90]. mannose [ITP90]. mannose- [ITP90]. Many
[KL91, Al95, BB99, FPC91, KO97, Z93, Zho93, ZL94]. Many-body
[KL91, Z93]. many-center [FPC91, ZL94]. many-electron
matching [MRM97, PS96b, SHCY93]. materials [BR97, GC98].
Mathematical [Cas89, Gar90, Jem97, PPK91]. matrices [Bal93, BB98b, BC95, BB96b, CMC92, GM90, GHR93, Mit94]. matrix [BH91a, BC96, BB98a, BoF94, CT95, CLCL96, CW97, FTW+96, GHR94, KTK93, KV93, LMB96, LH99, Mil90, ZL94]. matrix-inversion [CT95]. matter [CBS94]. maxima [Che95a]. maximization [CACD97]. maximum [J98]. MC [SS98a]. McLafferty [LP92]. McMurchie [Cis93].
membranes [SB99a, TM95]. memories [GW95]. memory [BDKL95, CS90, DK93, FK95, fGGG94, Lim97, LMCPP92, MD95, MOSD97, MTBS91, Ske91, CS96]. mercaptans [AF97]. Merck [Hal96a, Hal96b, Hal96c, HN96, Hal96d]. mercury [CY98]. Merrifield [Mez91]. mesh [BBR96, Bec99a, CF97a, LWNS95]. mesh-based [LWNS95]. Meshed [BH98a]. meshes [CF97b]. message [VM95]. metabolism [WM93]. metal [BCMZ99, Bér97a, BBCa98, DBV994, DBV98, FS95, GKK98, GSK95, LS98, LHB93, LJ92, LDJ92, MM93, Mag95, MK97, RCAA99, SH91, Yos90, dVM91]. metal-free [BBCa98]. metallofullerenes [NKA98]. metals [CH96a, HM90, HHC90]. methane [CY98, FS98b, MFG97, FS97, WM93]. methanes [WM93]. Methode [BF96, KPV96, PZBM98, ATK94, Aer95, AT93, AS98b, AB97, BRP92, BSS90, BB98b, BWS95, BG99, BBR98, BR97, ÇHP91, CR95, CLCL96, CT99, CCJ99, CT97, DBS91, DHHY90, DJ94, DBS93, DSB96, DKR95, Dum91, ELA95, ET98, FOCB96, FCNSA98, FRZ93, FPC91, FS97, FUS94, GKM94, MGL94, GJK93, GPF97, GGP96, GS94c, HBL98, HNS97, HK98, HK91, IC96, Ish98a, JLV97, Jon91, JDD97, JLN98, J93, KZ99, KMKW98, KID93, KTK93, KD96, KTh99, KK91, KRB92, KRB95, LL92, LSR97, LB96, LT91, LBO94, LAO96, LMFA92, LDM92a, LWS95, MK98, MM94b, M97a, M98, MJ93, MVS92, MJFT96, MR98, M98a, Mul91, NL91, NM97, Ni91, NWÅ95, OS98, PS96a, PNJS93, PKN95, P97, PH96, PN95, Pur98, RK97, RM91]. method [RW99, RE99, RCv96, R96, R94, RH90, RK90, RN90, SE95, S91, SQ95, She90, SMM97, SMF91, SNS95, SWK99, Ste90, SU93, SW96b, SB92, TH93, TKSN96, TRR94, TMC96, VSS96, VGN92, VTR94, VS97, WM95, WWXS97, WF94, WHHP97, YTT97, YL90, Y94, ZM90, ZV96, ZYY95a, ZM90, EKS97]. Methodical [KT93a]. methodological [Bog99]. methodology [CCBK95, CF94, SB98a, BJK95, DH95, MHS94]. Methods [MS98, TNKM91, WHHP97, vDrdV92, AB98a, AVP93, AJ96, Anc15, BCG97, BMK90, BR99, CT95, CW93, CMS91, CNK97, DV95a, DV95b, DN92, Fab91, FGBH90, FKN93, For91, FSI95, GH98, GJK93, GPPS91, GLoFP96, HL96a, HKS97, HS95b, HBR99, JJTP93, KS96, KCK98, LSD99, LHL95, Luk94, MK97b, MM94c, Mez91, Mit94, MM95, NBS94, OS94, OBL95, PS98, PT96, PAS99, PT98, RK97, Ric93, ST91, STB94, SW93a, SHT94, SHT94, SR98, SOL97, SHTC93, SB94, Ste91, SK93, TJ96, VRBE93, WV96, ZvN93, Z90, vFB91, DB98, NSWP90, Chr90]. methyl [BHK91, CK91, C91b, CG90, CG96, EnvRS94, HM91, HCC99, KSP90, LBB94, MS98, PG91, SMS98, dANS96]. methylalaninamide [SVS97]. methylamides [HMÇ91]. methylation [CP98]. methylbutyronitrile [CC91b]. methylcarbamates [Kat90b]. methyldioxidirane [ABBC99b]. methylene [Can93]. methylenecyclohexane [Jai90]. methylenecyclopentane [Jai90]. methylhydroxycarbene [NBG93]. methylinole [WLK92].
methylpterin \[CG96\]. methylsulfonyl \[SSQ92\]. Metropolis \[Dum91, JMH96, SS98b\]. Mezey \[BP93b\]. Mg \[GG96, Mar98, PFFF97, Ste91\]. microcanonical \[Dum91\]. microclusters \[Pul97\]. Microscopic \[LCW93, LW92\]. Miertus \[VWGF95\]. MIMIC \[MRM97\]. mimicking \[BPS93\]. MINDO \[FDMB92, KHF91, MFG91, VFM+90\]. MINDO/3 \[FDMB92, KHF91, Kas90, MFG91, VFM+90\]. mineral \[TYMS98\]. mineral/aqueous \[TYMS98\]. minimax \[Dum91\]. MM-EHMO \[IMP91\]. MM2 \[AYC94, CT97, FRC91, MSB95, MSB96, BW+90, Fro91, GPPS91, HMC91, Ja90, KHB92, Sau91, SGB91, SS93, SAF93, SMM90, SR90, TNS97a\]. MM2-87 \[Fro91\]. MM2/MM3 \[SGB91\]. MM3 \[ALS90, AF93, AF94, AYC94, Ay97, CRC97, FA94, LBB94, LCD+97, LA92, LA94, MSB95, MSB96, ALY90, DRF92, FD94, KPI95, ALY90, LFC96, LA91, LA98, Sau91, Sul95, TA98, TNS97a\]. MM3-MD \[LCA94\]. MM4 \[ACK+96, ACL96, AF97, NCA96, NA96, NGA96, TNS97a\]. MMFF \[Hal99b, Hal99a\]. MMFF94 \[BBH99, Hal96a, Hal96b, Hal96c, HN96, Hal96d, Hal99b\]. MMFF94s \[Hal99b, Hal99a\]. MINDO \[Fab91, FDMB92, FSI95, GJR91, HK+97, KHF90, KHF91, Kas90, Kat93, KWS99, KT93a, KT93b, LIO90, MFG91, LOR95, OBL95, PT96, PT99, Rod94, SUG92, VFM+90\]. MINDO-PM3 \[Fab91, Kat93\]. MO \[PSY+99, PK91, AC92, GPK95, MTR95, ST91, VK94, WHM+96, SR94b\]. MO-Studies \[AC92\]. MO-theoretical \[GPK95\]. mobile \[SB99b\]. mode \[FGGG94, KG91, KG99, SMM96, ZS93\]. Model \[TP93, ABE+96, BCT98, BRC94, BF96, BKM97, BSL91, CPR90, CHP91, CTC95, CT92, CG97, CG98, DVM93, DVL95, DVL90, DK97, DBV98, Fer95, FTA91, FSS97, FRZ93, FS98b, Gao97, GMM95, HS99, HCK95, HCC99, IRR93, JS93, Kat93, Kus92, KID93, KA96a, KTI93, KTn99, LMMRL98, LJD+97, MFG91, MNVM97, MRS98, OS91, O'm99, PK98, PTB99, PKK99, RC93, REA+98, RC99, RL95, SBB97, SSM96, SSR99, SCRI93, SK95, TSK96, TRG99, TRLRB96, VWGF95, Wib99, WPL95, XWS92, ZFY95, dVA92, AC92, MTR90\]. Modeling \[Her97, JKS93, PB92, PPAS+99, ATK94, Aer95, BW+90, BDH+94, BPZL96, BBC+98, BP94, CHP91, CHP90, CEA92, DP95, EHNW96,
EPBD95, FZL97, FM91, GC97, Jen94, LP95, MRG+90, PFMI97, PF99, PMRG93, RSOF96, RL95, TRJ96, TS99b, WC90. **Models** Cas89, Sie96, BRP92, BMN99, CJC+93, CMPT98, Cri95, Gar90, GHS97, HK90, HVvRS93, JB95, LHL+95, LW92, Mag95, MK92, MSZ96, PFC96, PF91, RC95, SC99, SLH96, SKOR93, TD95, TS90, WS99a, WO97, Wil94, WA99, WWF95.

**Modern** Yar95, KLR96, Dav97.

**Modes** DOO93, DZ97, GW98c, KCK97, TRG99, ZS99.

**Modifications** AJ99a, AJ99b, KRL+93, SMA92.

**Modified** IRRR93, SAF93, DS92, FA94, FR90, FRC91, Fro91, GS90c, GMM95, GHR93, GBT97, HS93b, IMP91, LB96, LA90, LHB93, LH96, LBB94, LJL98, LBI+97, LMCPP92, LA94, NCA96, NA96, NA96, NQ99, NSWP90, Ob98, OL93b, OC98, PKCM99, RvRS98, SBA97, SB98b, SB98c, SKB92, SB92b, Tax99, TYS998, VH99, Van97, VRC92, WC90, WLK92, YKU96, Yos90, vOC93, AM99, Aer95, AT93, AGP91, AL93, AC92, ALO94, AVA93, ACK+96, AFK+95, AS98b, AHRL+91, Art93, AW90, BT96, BCB+97, BCT98, BLKS95, BO93, BDK+94, BRC94, Beck97, BFR93, BvGMP97, BWS+95, Bic99, BS97, BPZL96, BG96a, BK96, BCT91, BV97.

**Molecular** AL90, AYT90, AF93, AYC94, AF97, ACDP98, BBR96, BB96a, Bla91, BCB+98, BCF+92, BL91, CLCL96, CW97, CP98, CB97, CH88, CG98, CS92, DM91, SFA94, FR90, FRC91, Fro91, GS90c, GMM95, GHR93, GBT97, HS93b, IMP91, LB96, LA90, LHB93, LH96, LBB94, LJL98, LBI+97, LMCPP92, LA94, NCA96, NA96, NA96, NQ99, NSWP90, Ob98, OL93b, OC98, PKCM99, RvRS98, SBA97, SB98b, SB98c, SKB92, SB92b, Tax99, TYS998, VH99, Van97, VRC92, WC90, WLK92, YKU96, Yos90, vOC93, AM99, Aer95, AT93, AGP91, AL93, AC92, ALO94, AVA93, ACK+96, AFK+95, AS98b, AHRL+91, Art93, AW90, BT96, BCB+97, BCT98, BLKS95, BO93, BDK+94, BRC94, Beck97, BFR93, BvGMP97, BWS+95, Bic99, BS97, BPZL96, BG96a, BK96, BCT91, BV97.

**Molecular** BS97, BGZP97, BW90, BP94, BR90, CZM98, CPR90, CDG+99, CHF90, CA93, Che95a, CC98, CCJ+99, CRP97, CK91, CACD97, CMS91, CMC96, CT97, CT92, CC91b, CH94, CH96b, CG96, CG97, CG99, DM94, DOO93, DDDV93, DDL95, DK93, DRC96, DVL90, DHH90a, DV99, DK97, DA96, Dun90, Ear93, EGH+93, EGHT97, EA93, ELA+95, EPBD95, EK97, FSW96, FHB99, FCNSA98, FK91, FGG+92, FB90, FW93a, FLHP97, FLP98, FG96, FW91, FPC91, GGG98, GPSS93, Gen99, fGGG94, GS90b, GCT96, GC97, GC98, GGP96, Gre95, GG96, GJD94, GT98, GH97, GPPS91, GLoNP96, Hal96a, Hal96b, Hal96c, HN96, Hal96d, HS93a, Har93, Har99a, HCT98, HGB93, HW97, HE99b, Her93, He97, HYA92, HBB97, HEN+94, HYH+94, HS95, HK91, HCK95, IG94, JF92b, JVB95.

**Molecular** JM90, JG93a, JS93, KR96, KLV94, KRM92, KLR96, KWS91, KWH+90, Klo92, KE95, KUT+97, KHB92, KB92, KVKK93, KKCH96, KKJ97, KHK96, KPR91, KTS92, LDPV91, LM93, LK95, LKL95, LPK99, LCA94, LLD98, LCD+97, LA92, LP95, LS94, LI90, LO98, LWS+95, Mag93b, Mag93a, MK98, MTH94, Mar97a, Mar97b, Mar98, MI99, MM95, MV91, Maz97, MJ93, MS95, MSB96, MK97b, ML91, MTBS91, MSCP94, MRM97, MM94c, Mit98b, MRG+90, MN95, MBP98, Mul91, NBS94, NTK96, Nic97, NM97, NWAM95, NL98, ORK+91, OS98, OS94, OL93a, OM96, PPK91, PPK92, PK98, PKRR97, PA90, PaST94, PMIB99, PSY+99, PGBM97, PZBM98, Pet95, PG91, PB92, PPAS+99, PS96b, PH96, PFL93, PE92, PT98.
molecular [RD97, RMS93, RHKK90, RSK92, RTSM93, RKL93, SSD93, SADV97, SBB+93, S993, SN99, SHCR97, Sha91, SWM90, SM94, SN91, STPA91, SB99a, SK99a, SACK95, SB90, SM94, SM90, SK92b, SYHW99, SL95, SR92, TH93, TMB93, Tav96, TRR+94, TRG99, TRJ96, TvG94, TMK+99, TMCM+96, TWR+95, TNS97a, TNS97b, UF93, VP94, VWF95, VRC91, VPV91, WAM91, Wan91, WWSS98a, WWSS98b, Wel90, WS92, WA99, WPLC95, WAW+97, WKP+90, WN91, YC95, YL90, YB94, YB95b, YTRB97, ZHS92, ZM90, Zau91, ZYY95a, Zho93, ZL94, ZG92, Zim91, CB94, Hal96c, RJP97, SB98b].

molecular-field [MRM97].

molecule [AC94, Bro99, Kri90, NSA+97, RPR+98, TKTN99, TMCM+96, YB95a].

molecules [AS98a, ASM+92, BLO94, BF93a, BW91a, BM97, CNOJ93, CW91, CASC96, CACD97, C99, CG97, CG99, DF97, Din91a, Din91b, DJ94, EPW97, Fab91, FPL95, FW92, FRZ93, FS97, GM90, GJK+93, GP94, GW98c, Gri94, GSW90, HBL98, HG93, Hi98, Hea90, HK95, HMS93, HJB96, JTP93, JTM+95, JS93, KG92, KD91, KJ97, KG93, KHA90, KSD90, LSCA98, LDP90, LL92, LKLB+99, MAP97, MK98, MI98, MRG+90, MPJC98, Net94, NV+97, OJL93, PNJS93, PK95, PRR97, PH94, Ph90, PC94a, PD99, RCB99, RRR92, ST91, SC94, SR94a, SS98a, SS95, SACKH95, SWAH91, TKF92, Tel90, TG98, TGW96, TJP96, WAM93, Wan97, WHF97, WS93, WCMS91, ZV96, vEK99].

Møller [BCFM98, Klo94, RPW98]. Molsurf [NS98]. molybdenum [Van97].

moment [LP95, McD96, SB91]. moments [BRC94, Din91b, GM90, K95, RSK92, SR98, SS92, SACK95].


monosubstituted [SK91, Van97, VFM+90]. Monte [Dum91, J98, JMJ96, SS98b, BM90, CF97, CE96, CCJ+99, CBSB94, CLO99, DBV98, DN92, DY97, ET98, FB97, FCS98, GLP95, GPB+97, GVH94, GLOOB91, GS94c, GBE92, HL96b, HNS+97, HHP91, JG93a, JN93, JLNTR93, JAd96, KID93, Knu90, Mar90, MM97, NBS94, NV91, PK97, PLB92, PH94, RPG+95, SS98a, TM95, TS99a, TMCM+96, VGN+92, vFB91].

Mori [MN92]. MORMIN [PGAL93]. Morse [DKK+93, DKK95]. most [PP97, RTSM93]. motion [DOO93, Dr94, Maz97, Mil90]. motions [EPBD95, Gen99]. MP2 [BvH+92, CW93, FV98, HA93, Lim97, MD95, PS98, VHV90]. MP2-energy [Lim97]. MPGRAD [HA93]. MPSim [LBI+97]. MRCEPA [VVSV96].


N [Ano97, Ano15, BvH+92, GBT97, KTT94, KTT95, SVS+97, KTT94, DJ94, GM98a, HMČ91, HDA93, KTT94, KTT95, McD96, PT99, TK94, VTR+94].
N- [HDA93]. N-NMR [GM98a].
N'-tetramethyl-P-diaminobenzene-chloranil [KTT94]. N16 [CBSR99].
neolignans [CT97]. neon [MN95]. neopentane [MFG97, PCKM99]. net [PNJ93, PKN+95, Su93, Wil94, WK5+90]. network [KD96, MK94].
Newton [AB97, DZSB94, SB90, ZKA94]. Newtonian [PGAL93]. Nguyen [Ano15].

[BMW+90, Cul92, GZ95, JZ96, LS98, RBC+98, SV94, SCZC99]. **pairing** [PD99]. **pairs** [Pra93, RC95]. **pairwise** [DH90b, WSS99a]. **palladium** [Sel90]. **Palmitoyl** [LH96]. **pancreatic** [Kik96, PS92]. **papain** [KR96]. **paperback** [Dav97, Dav97]. **paracyclophanes** [BRLD92]. **Parallel** [BCFM98, BHE+93, CBWF98, DKH98, GF96, LWNS95, Lim97, MD95, MOSD97, NIS98, Net94, NS95, PLY98, VT91, BBR96, Bec97, BDKJL95, CDG+96, CMC92, CS90, CS96, DLS+97, DPK94, FK95, GJL+90, HL96b, JF92a, JP92b, LB1+97, LMFA92, MTBS91, PH96, RGK93, RBC+98, RBE98, SS93, SLG93, SOCF98, SWK99, SL95, TMK+99, VM95, VA98, WHHP97, WH95, YB94, JP92a, JP92b]. **parallel-coordinates** [Bec97].

**Parallelization** [JG93a, KMO92, DK93, TA94]. **PARAM** [SLG93]. **paramagnetic** [Kar99]. **Parameter** [LFB96, BSV94, CA95, ISH98b]. **Parameterization** [Fer95, CT92, FSBMP99, GH98, Hal96a, LA90, LBB94, LFB96, NL98, SGB91, LPW+97]. **parameterized** [TRLR96].

**parameters** [AJ99a, AGP91, ACFO91, AKF93, BLO94, BCB+97, Can93, FG96, GDK92, Hal96b, Hi97, HH99b, KT93b, KHB92, LOP+97, MTRJ95, MRH99, NWAM95, Ran91, RSB96, SEJ95, SB95, Smi99, Ste91, SWAH91, SK95, VFK92, WH93, YB94, LDLV95, PT99]. **Parametrization** [DMV98, FR94a, HLO99, OM96, Hal96b, HA95, HH99b, KT93b, KHB92, LOP+97].

**Parameterization** [DOO93]. **partition** [BH91b, Kw91b, Tru91]. **Partitioning** [DOO93]. **passing** [VM95]. **Path** [Mor93, MN95, Bau90, DBS96, Mez92, PB92]. **paths** [HH99a, ZMC+97].

**pathway** [VP94, ZVP98]. **Pathways** [SR92, AJ89b, Sau91, VP92]. **pattern** [CBR97, Mar90, SHCY93]. **Pauli** [Cha92]. **Pb** [JFR92b, Ste91]. **PC** [Rog90, Rog94, Rog03]. **PCs** [TRJ96]. **peak** [CCN90]. **PEFF** [Dil92].

**2-pyridone** [RGK93]. **6-31g* [FW93a]. **AMPAC** [LW92]. **aqueous** [TYM99]. **CHARMm(R)** [MR92]. **chloroform** [VW96]. **density** [RW99]. **empirical** [YM98]. **energy** [GBE92]. **equatorial** [CP98]. **formaldehyde** [MP90]. **grid** [LWS+95]. **M** [Mar97b]. **MM** [CG97, CG99, Gao97, LO98, PF99]. **MM3** [SGB91]. **molecular** [FCNSA98, SHM95]. **Monte** [MJSV92, SMM97]. **MST** [LB094]. **oligoazine** [SE94]. **quantum** [BvGMP97]. **rapamycin** [SS94]. **SA** [REA+98]. **SCRF** [LBAO96, OJL93, OBL95]. **stochastic** [GS94]. **surface** [NSB94]. **Vis** [BMD99]. **water** [DN92, SB99a]. **Penning** [CC98]. **penta** [TRG99]. **penta-** [TRG99]. **pentagon** [AOY96]. **pentahalides** [BT92]. **pentanes** [GdAG+98]. **Pentium** [TR96]. **Pentium-based** [TR96].

**pentynne** [CC91b]. **peptide** [BSL91]. **Peptide** [GVD96, PFC96, BPS93, BK97a, Bec97, Büh99, Dav94b, GS90c, HO93, HS95a, JLIW97, KOH98, KFMM99, MTRJ95, Par99, PMIB99, RK95, SS98b, WP97]. **peptides** [AC92, AS96, BCB+97, BM99, BMN99, Dav93, Dav94a, GS90a, GS90b, HYA92, KF99, MNH+98, MM97, NTK96, SKOR93]. **Pepto** [CCN90]. **Performance** [BMN99, DNC96, HKS+97, SKT94, VA98, FTW+96, GM98b]
proton-transfer [LMRRL98]. protonated [LCD+97, NBG93, ZCP98].
Protonation [HOL98, RTGJ98, Wel90]. prototypes [GMY97]. proximity [SSV93], prudent [HKK91].
Pseudopotential [KSP90, JFR92a, JFR92b, SS95, VSF97]. pseudopotentials [SRI92]. pseudospectral [BCFM98, CBWF98, KZ99].
Pseudopotential [KSP90, JFR92a, JFR92b, SS95, VSF97]. pseudopotentials [SRI92]. pseudospectral [BCFM98, CBWF98, KZ99].
Publisher [Ran92]. Publishers [Var92]. Publishing [Dav97]. pulse [FR90].
PVM [SL95]. PVM-AMBER [SL95]. pyrazole [LSFFM+95]. pyridines [BHK+91, SK91]. pyridone [RGK93, BA94]. pyrimidine [WMM+95, Wun92].
quadrupole [Din91b, EGH+93]. qualitative [RK97]. Quality [KNST96, RWB99, BPP90, RC93]. QUANTA(R) [MR92]. Quantification [WTLC93]. Quantitative [Ric91, RMS93, CSC96, CS95, DJ92, DKBS97,KF94, Mar90].
quantitatively [GW98c]. Quantum [ACD97, DV97, ENH98, FCNSA98].
quasirigid [BH98a]. quaternions [SA99]. Quinhydrone [KTT94, KTT94].
quinone [AF94, Ano97].

R [Dav97, Mez91]. Radial [PG98, ABD+98, ZY96]. radiation [WM91].
radiation-induced [RMW91]. Radical [GCC97, GM98b, Bau90, Cai94, FSS99, FOA98, GMO93, ISH98b, Kar99, LP92, O’99m, Ove91, VKC96].
Ramifications [UF93]. random [BW96, FR90]. range [Aqv96, ADG99, BPC91, LOP+97, LPW+97, Ric93, SB94, TMB93]. rank
[Mit98b]. rank-one [Mit98b]. Raphson [AB97, SB90, ZKA94]. Rapid
HG93, HK92, Ish98a, LM93, NTK96, EGHT97, FW93a, GS94b, MKS97,
NH91, PCG+92, SNS95, YB95a, LDM92a]. rapidly [GS94c]. rare
[BBS96, WH93, Lóp95a]. Rare-gas [Lóp95a]. ras [YSJ95]. rate
[Dum91, DBT98, MGLL99, Phi90, Pol90, YC95]. rather [vRSD92]. ratio
[SN90]. Rational [LJKL98, Tay99]. rationale [SSM96]. Rationalizing
[FM94]. rattle [FS98a, FS00, MK92]. ray
[BSL91, KRL+93, PS91, PS92, SYHW99, WJL+96, WJ+96]. reaction
[AC92, AJB96, AIDAV98, ARLG+94, Bau90, CLS+97, DJV+95a, DJV+95b,
DBS93, DBS96, FW92, FA99, FOA98, FUS+94, FS95, GLLOB91, HOL98,
HB91, IBkV-R92, JZ96, KCK97, LMB99, LV90, LS94, LSSvRS96, LDMS99,
MGLL99, MRS98, NVER97, PLB92, PB92, RRR92, SBM97, SS97, VP92,
VP93, VP94, Vas92, WO97, ZVP98]. reaction-diffusion [Vas92]. reactions
[CG90, GCRSAIVB99, GHS97, JB98, JKN99, LKL95, LS98, LDJ+97, OS91,
SMA92, SSV93, SWOW97, Vya97, ZMC+97]. reactive [SB98a, TRLRB96].
reactivities [BH98b]. Reactivity [BHK+91, SS97, Bic99, BS99, Che99,
ISH98b, JFFK94, LQ98, OR93b, SSM96]. real
[BC93, CMC92, Mit94, SCC93]. realistic [PDP97]. Realities
[Cas89, Gar90]. realization [WWZD92]. Rearrangement
[CLQSS98, Bau90, HY96, LP92, RJP97]. rearrangements [KW91a].
recently [DHHY90, HO97, Ste90]. receptor
[AT93, AV93, AHL+91, CA95, GH98, LK92, LWS+95, SQ95, ZS99].
recipe [Klo97]. recognition [CBR97, Mar90]. Recommendations [Pol93],
Reconsideration [SKK+93]. reconstruction [MKS97, RS92]. recurrence
[RKL93]. redox [CG90, TYRD92]. reduce [DB98]. Reduced
[TWR+95, AB97, BHK+91, BS94, QHIH98]. reduced-parameter [VS94].
reduced-restricted-quasi-Newton [AB97]. reductase
[CG90, CG94, CG96, CG98, LK95, We90]. reduction
[Bru93, WWS98a, WWS98b, fGGG94]. reductive [WM93].
redundancies [PPK92]. redundant [PAS96]. reevaluation [SSV93].
Reference [RLA+98, KTnH99, RSK92]. refine [MKS90]. refinement
[Bec99a, GKM94, GF96, LBF96]. Refinements [FTA91]. refining
reformulation [AB98b]. regiochemistry [CN98]. region [DH99].
Regioselectivity [NVER97]. Registration [PS96b]. regressions [Ran93].
Regression [DMB91]. regular [GS94]. regularization [SB92]. related
[AF94, Ano97, Din91b, G90d, Gr90, LPP99, LS98, Mag95, MHJ+98, MR93,
MGPR90, RdBN90, SD98, SSV93, SB92b, WO97]. relating [Kna92].
Relation [McD97, SG95]. relations [MGH97, RKL93]. relationship
[KF94, Pao90, Par99, Ran91]. relationships [DJ92, GLLOB91]. Relative
[CGBC96, DN92, Fr93, BSC+98, BSvRS95, CK91, CG94, ER95, HCK95,
LS96, RE99, SVM99, SCP92, SACKH95]. Relativistic
[Dya98, ES99, HOL99, Kut99, PC94a, SCMV97, Van99, EBD+99, FV98,
HKY98, Klo97, LL92, VES+99, SI93, Van97]. relaxation
[NH91, SHCY93, WPLC95, ZRVD93]. Relaxed [TP90]. relevant [Gre95, GG96, ZM92]. Reliability [SRI92, BKL+90, LI90]. Remarks [CT95]. renormalization [CT95]. Reorganization [LH99].

reparametrization [MFG91]. replace [FK91]. Replicated [WAW+97, YB95b]. Reply [St90]. represent [Wi94]. Representation [TKF92, CZM98, CL99, DH94, FS91, KKE93, LMB96, LBO94, Pac93, PWS96, Bé97a, TKSM96]. representations [BSV94, GKS93].


series [Fer91, Gre95, KMM99, Kea90, Pol90, Ran93, ZY96]. set
[AG90, AW91, BPP90, BR97, BBH99, CDG+99, DF97, FG96, GC97, HVM99,
HK95, IS91, JDD97, LMA99, PAS90, SBA97, SS97, SB92a, WB91]. sets
[Als95, BW91a, BC90, CRME93, CB96, CH96a, DM94, GvRSvEH+93, HM90,
JG91, JLN98, KNST96, MH97, RW99, REA+98, SH91, SR92]. Settle
[MK92]. several [BL91, DV99, FR90, GLoNP96, RMS93, SBA97]. SH
[CC97, SS95]. SHAKE [DKRK95, FS98a, FS00, MK92]. Sham
[Abc99, HT99a, SBA97]. Shanno [AB98b]. Shanno-like [AB98b]. Shape
[Art94, WAM93, Art93, GGP96, MTH94, PZBM98, SKB92, WAM91,
WMM+95, dVa92, WMM+95]. shaped [FM99, SD98, TG98]. shapes
[Bek97, COR99, WAM93]. shared [Lim97, MTBS91, Ske91].
shared-memory [MTBS91, Ske91]. shell
[ACD97, BCB+97, Cha92, HBLL98, LLB99, PG98, PC94a]. shells
shieldings [FGBH90]. shift [CW91, GM98a]. shifted [DKBS97].
shifted-force [DKBS97]. shifts
[BH98b, BKMM99, GP94, IBKvRS92, KMM99, PT99, WHHP97].
shotting [KT93]. short [ADG99, GVH94, LPW+97, PS92]. short-range
[ADG99, LPW+97]. shorter [RHN94]. should [Jai90]. Si
[CLS+97, JFR92b, BKMM97, IRR93]. SICI [Ano15]. side
[KS97a, Dav93, HM91, KDF96, LOP+97, TEHL93]. side-chain
[KD96, LOP+97, TEHL93]. signs [SF91]. SiH
silicide [UVRC97]. silicon
[ACRC97, CJC+93, CJC+96, CJC+96, MRW91, RMW91, VW91]. siloxanes
[Ear93, KHG96]. silverware [Bla91]. SIMD [RBC+98]. similar
[GW98c, Par99]. similarities [CSC96, MSDC94]. Similarity
[ZK93, ACD97, ACDP98, ACD99, BP93a, BRH90, CACD97, KRL+93,
MK98, MK97b, RM97, PRR97, Pet95, Pet93, PS96b, WM95, JM90, Klop92].
Simmons [Mez91]. Simple [Ano15, BG99, BZP97, CNK97, Klop97, SS98a,
BP98, CHSK96, ETA91, GPG96, IS91, KT999, LKl+97, MSZ96, Mul91,
PN95, Tru91, VRC91, VRC92, WS99a, ZYY95a]. simplex [FSB99].
simplified [FS91, KK91, KTK93]. simulate [PDP97, Z93]. simulated
[BM99, CE96, EHNW96, GW95, MPBM98, NVS91, Ni91, Sn92, WP97,
WCS91, YTT97, Lim97]. simulated-annealing [NV91, Sn92].
simulating [For91]. Simulation
[CJC+93, CJC+96, LMB99, AGP91, BS+97, CB94, CCJ+99, CBSB94,
CG93, CHSK96, DS92, El91, GPB+97, GMM95, GLLOB91, GS94c, GK93,
HS93a, HS93b, HL96a, HL96b, HR97, HBR+99, JG93a, KUT+97, LB96,
LH96, MTBS91, Mor93, MJSV92, NBS94, NQ99, OC98, PSW96, PMIB99,
PL92, PH96, RE99, SB98a, SN99, SWM90, SN91, SB99a, SB94, SYH99,
SJ95, TCM+96, WWXS97, WSV92, WAW+97, WS98, YK96, TM95]. Simulations
[CP90, SWAH91, YBD+94, AKF+95, AW90, BCB+97, BO93, Bek97, BvGMP97,
BSL91, BM90, CG96, DOO93, Dav93, DKRK95,
EGH$^+$93, EGHT97, EJ95, FB97, FHB99, FOCEB96, FBK90, GLP95, Gao97, GVI94, GDK92, GT98, HYA92, HBBF97, JN93, JLNTR93, JJ98, KHW$^+$90, KVKK93, Kuc96, LPK99, LCA94, LOP$^+$97, LPW$^+$97, LKC$^+$98, Mar90, Mez92, Mez97, NSWP90, OS94, OM96, PHG94, SS98a, SKT93, SKT94, SMA92, SWOW97, SK92b, SW96b, TMB93, TYMS98, TMK$^+$99, TSN97b, VWGF95, ZS99, Zau91]. simulator [Zim91]. Simultaneous

[LMB96, Kea90, NL98]. SINDO1

[AJ99a, AJ99b, GJ95, JG93b, KJ97, LJ92, LDJ92]. single

[VGH94, HM92, SVM99, TK94, WJL$^+$96]. single-stranded [VGH94].

singlet [KHF91, LDJ$^+$97]. singlet-triplet [KHF91].

singularities [BK96, EA93, GO95].

SiO [AS98a, KHG96]. Site

[WA99, Cri95, CG96, GKM99, TK94, WJL$^+$96]. single-stranded [GVH94].

singlet [KHF91, LDJ$^+$97]. singlet-triplet [KHF91].

slater [CDG$^+$99, Jon91, RLA$^+$98]. Slater-type [CDG$^+$99, Jon91, RLA$^+$98]. slow [LMB99].

SM3 [CT92]. Small

[SG95, APC98, DF97, DBS91, DJ92, LDJ97, LPW97, LKC98, Mar90, Mez92, Mez97, NSWP90, OS94, OM96, PHG94, SS98a, SKT93, SKT94, SMA92, SWOW97, SK92b, SW96b, TMB93, TYMS98, TMK$^+$99, TSN97b, VWGF95, ZS99, Zau91]. simulators [Zim91]. Simultaneous

[LMB96, Kea90, NL98]. SINDO1

[AJ99a, AJ99b, GJ95, JG93b, KJ97, LJ92, LDJ92]. single

[VGH94, HM92, SVM99, TK94, WJL$^+$96]. single-stranded [VGH94].

singlet [KHF91, LDJ$^+$97]. singlet-triplet [KHF91].

singularities [BK96, EA93, GO95].

SiO [AS98a, KHG96]. Site

[WA99, Cri95, CG96, GKM99, TK94, WJL$^+$96]. single-stranded [GVH94].

singlet [KHF91, LDJ$^+$97]. singlet-triplet [KHF91].

small-amplitude [SG95]. smart [SS98a]. Smoothing

[PP97, BNDS97, DM91]. soft [Kul90]. softness [CN98].

Software [TS99b, MK94, MRG$^+$90]. solid

[Kul90, NQ99, Tav96, Vva97, WTL99, DBS91, FB97]. solid-state [Vva97]. solids

[DKBS97, EBD$^+$99, NBB$^+$99, Ste98]. soliton [För92]. solubilities [Her93].

solute [BL90, FS97, KOH97, Mez97, YB95a]. solutes


[AS97, Bla91, Cis93, CG93, DM91, JKN99, LW92, PR90]. solvated

[ARLAB99, LBO94, RRR92]. Solvation [KJ97, MRS98, REA$^+$98, Smi99, Art94, CFK97, CT95, CBT94, CK91, CMPT98, CT92, CG99, FTA91, HL96a, HY96, Her97, KOH98, LW94, LHL$^+$95, LW92, PT98, Pur98, RE99, SH98, SK95, VWGF95, WWXS97, WWF95, dVA92, AVP93]. solve [NH91].

Solvent [CG96, MRH99, SJDW90, WCK96, ACB97, ARLG$^+$94, BFH94, CTC95, CLO99, DF97, FRZ93, FDR93, FS97, Gao97, GMM95, GO95, LD92a, PSK98, PaST94, PLB92, PM93, PKCM99, SAdV97, Sh91, SNS95, SKK$^+$93, VS97, WSS99a, WSS98a, WSS98b, WSS99b, WSS99c, YB95a, ZKS93]. solvent-accessible

[FS97, GO95, WWSS98a, WWSS98b, WSS99c, ZKS93]. solvent-excluded [GO95]. solvent-excluding [PaST94]. solvent-inaccessible [WSS99b]. solvents [LBA96]. solver [HBBF97]. Solving

[LD92b, ZYY95b, Ram90, Wan91]. Some
Strength [AJ97, CTJ+94]. stretching [OL93a]. stringent [Tel90]. strong [GSW90]. Structural [AGN+90, GG91, LHB93, MGH97, SV94, SUG92, AS98a, Gri90, Kea90, MvRSL+97, NKA98, VP93]. Structure [ARLAB99, CER94, Dav97, GYT+98, ATK94, Arn94, BSGB98, BCFM98, Bog99, CBWF98, CNS96, CJC+93, CH96b, DNC96, DKJ96, DJ92, DS90, DRP98, DN92, EKS97, FRZ93, GF96, IG94, Jen94, JMH96, KR96, KRM92, KW91b, KP94, LS98, LWNS95, LOP+97, LP+97, LKC+98, López95a, López95b, MM93, MKF+97, MS95, MvEP+98, MTR90, ORK+91, PG98, PL94, RdBN90, Rat91, Ric91, SBB+93, SEJ95, TAC98, VK97, Van97, VTR+94, Ye95, YBD+94, ZM92, ZM99, vEK99, HBR+99, PY+99]. structure-activity [Ric91]. structure-property [Ran91]. structured [YB94]. Structures [ENvRS94, RCATD96, TNKM91, AB98b, BCT98, BMD99, Bec97, Bof94, BC95, BV+92, Che95a, CNS96,DrvSH94, EN98, EHNW96, GS94a, GC98, HBL98, HDA93, KG92, KFM99, KA96a, MI99, MM95, NV91, Obe98, PS91, PS92, PL94, PPK91, PR98, P92, PE92, SCP92, SB98b, SC91, SB92b, Sun94, VP94, VK97, We90, W93, WPLC95, VF92]. studied [BO93, HY94, KR96, SWM90, WJ+96, WJ96]. Studies [AC92, Dun90, AF97, ACPO98, BRD92, CR97, CG91b, EN98, FW91, GP93, Gr94, Ha99a, HK97, HR97, JFR92a, JFR92b, Kat90b, KWW98, Kh93, KCK97, KA90, LK90, LH96, LY95, LMA99, LO98, MS98, O'm99, Ric91, SB98b, SB98c, SUG92, SF96, SB92b, TA98, VH92, We90, WC90, ZVP98, ZMC+97, vOC93, LCA94, SW93b]. Study [Kik99, Sa97, ZM92, Zho93, ZL94, ACB97, ALPH91, AGN+90, AC92, AV93, Arn94, BSGB98, BA94, BPZL96, BKM97, BL90, BT92, BHK+91, BS99, BH99, Ca94, CLQSS98, CA93, Che95a, CK96, CAC99, CLS+97, CH94, CER94, CH96b, CEC97, CG90, CG98, CY98, DLM+98, DK96, DH90b, DKBS97, ER95, FF93, FVR92, FA99, FSC99, FLP98, FO98, GCRSAIVB99, GJ95, G90, GS90d, GPK95, GJ93, GJL+90, GH97, GBT97, HL96a, HRE98, HLO99, HK95, HMC91, HN91, IBK98, JT95, J96, JZ96, KS91, KW91a, Kar99, Kat90a, Kat93, KMM99, KRM92, KP99, KP94, KA96a, KHB92, KKH96, KH96, LK95, LKL+97, LS98, LS94, LDJ+97, LSSvRS96, LDM99, LO90, MP98, MI99, MS98, MTR95, MV91, MS95, MP90, NV91, NA97, NBB+99, NW95, NB98, N98, NER97, OL93a]. study [OL93b, PS98, PG91, PC93, PC94b, PFM91, PS97, RdBN90, Rat96, RJP97, RCB99, RCATD96, RR92, Rod94, RK95, SM96, SE94, SHB93, SR94b, SL+90, SSF90, SHI90, SVS+97, SRS94, SR92, SK91, TM95, TYR92, UVCR92, Van97, VRC91, VRC92, VPV91, VCLB92, VK96, VK94, VL90, VFM+90, WHM+96, WN91, ZBM91, GJK+93, TJ96, TRL96]. studying [FR94a]. subspace [IC96, KT99]. substances [Gr90]. substituent [ISH98b, KHF90, KHF91, SL+90, WTL93, PC94b]. substituents [ENvRS94, SMF91]. substituted
[AHLR +91, BCF +92, BHK +91, CPS90, GC98, JN93, JLNTR93, KHF90, MP98, PC93, TDFdc91, WM95, ZLM92]. substitution
[ČTS98, GG91, HKK +97]. Substrate [BO93, CFK97, SMA92, WNW91]. substrates [CG90]. subsystems [PS97]. successive
sums [CCG97, KVKK93]. Superacidity [BKK +96]. supercomputer [SOCF98]. supercritical [MSZ96]. superior [Cul99]. supermatrix
[CLCL96, CW97, YG92a]. supermolecular [Gre95]. supermolecule
[GG96, HY96]. supermolecule-polarizable [HY96]. superoxide
[SWM90, SWS +90, SMA92]. Superposition
[NVK +97, AG90, HVM99, Kca90, WB91, CACD97]. Supplementary
[Mag93b, Mag93a]. support [Fel96]. supramolecular [JMH96]. surface
[BG96a, BG96b, BKM97, BR97, CZM98, CT95, CP98, CS95, CLS +97,
DrRSh94, DS90, EA93, ELA +95, FB98, FS97, GÖ95, Her93, Her97, HREK98,
IBKvRS92, LM93, PAS90, PaST94, PCG +92, SS98b, SNS95, SBS99, SVS +97,
TA94, VB93, Wan91, WL91a, WWS98a, WWS98b, WSS99c, ZM90, ZYY95a]. surface-derived [SBS99]. surfaces [AV93, AB97, AHLR +91,
BW91a, Bec98, BJ94, BG99, CHP90, CMC96, DA96, FD91, HGB93, IRR93,
ITP90, Jen94, JAdV96, JKN99, LMA99, MTH94, PFMI97, PFF97, PAS90,
PaST94, PFC96, Pet94, PT98, QHII98, RK99, SB98a, Sa91, STPA91, SB90,
SC95, WAM93, WSS99a, ZHSB92, ZKSB93]. Survey [SHM99]. switches
[AM99]. sybyl [GJK +93, TJ96, GPP91]. Symbolic [Jem97, JK98, HB91].
symmetric [CML92, KA96b, Mit94, Mit98b, SA99, SMS98]. Symmetry
[Ste98, CHP91, CLCL96, CW97, Ear90, fGGG94, RCAA99, SA99, YKU96,
ZL94, ZM99, CLCL96, CW97]. symmetry-adaptation [ZL94]. Symmetry-matrix
[CLCL96, CW97]. symmetry-supermatrix
Synergy [BSL91]. synthesis [Dav94b]. synthetic [CT97]. synthetical
[ZKSB93]. System
[Gar90, BSN99, CCN90, CF97a, DN92, FF93, KKE93, LFB96, MRG +90,
MR93, Ram90, SOL90, SBB +93, SE94, SB99a, TEdV90, Vas92]. Systematic
[KMKW98, ZYP98, BT92, GS91, PFC96, dVA92, PS92]. systems
[BFH94, BWS +95, BJ9K1, CHPK91, Cso93, DF96, EKS97, EA93, FB97,
FHB99, FRXSR92, FGG +92, For96, GMY97, HVvRS93, Her97, IS91, JB95,
JVB95, Jen97, Kar99, LMB96, LBI +97, Lóp95a, Lóp95b, LLB99, LBO94,
MTR95, MSDC94, MFG97, Mor93, MPJ98, Mul91, MR93, MGPR90,
PHG94, PH96, PDP97, SSM96, Se90, SAF93, SEH95, SQ95, SM91, SCR93,
SKM94, TRR +94, TEdV91, TNS97b, WM95].

T [Dun90, Tay99]. T1 [SI93]. T3E [SOCF98]. T4 [EHNW96]. tables
[HC96, LM93, LB90]. Taiwan [SYHW99]. taken [VSF97]. Tanford
target [SF96]. Taunton [Dun90]. Tautomeric [Fab91, CAC99].
tautomerism [Rau96, RGK93]. tautomerization [LKL+97]. tautomers
technique
[Dav94a, FPL95, GS90b, Jai90, MGPR90, SJ95, TedV90, TedV91].
Techniques [Bak93, Dya98, SCC93, Bec99a, EKS97, FR94b, GBE92, KR96,
KPV96, PP97, SS93, SM91, VDF+97, WSV92, WAW+97, ZS93]. TeCl
[KCK98]. TeH [SS95]. tellurium [Klo93]. Temperature
[JJ98, AW90, FCS98, Gr90, Vya97]. temperatures [BK97b, JJ98]. tensor
[GDAG+98]. tensors [BSB+97, VES+99, ZM99]. terminal [YS95]. terms
[DV98, GS90a, KLR96, LPW+97]. terphenyl [OC98]. tetrahydroazepines
[AVC93]. tetrahydropyran [ZLM92]. tetramethyl [KTT94, KTT95].
tetramethyl-P-diaminobenzene-chloranil [KTT95].
tetramethylammonium [PKCM99, PBS97]. tetramethylene [GJ95].
tetraoxa [SHH+90]. tetrapeptide [PF99]. tetrodotoxin [Pet95]. thallium
[SI93]. their [Arn94, BRLD92, FB98, Gla90, HK95, HMC91, KPR91, LS98,
LHRF93, MFC91, MM97, PS97, PCG+92, SCZ99]. theorem
[GM98b, LJ91, ML92, HM92]. Theoretical [ARLG+94, BP93a, BSvRS95,
BRLD92, BH98b, Bii99, DLM+98, DBS96, FVR92, FM99, FDM92,
FDM93, FOA98, HKE98, JER92a, JER92b, JU91, Kat90b, KKKH96,
LK90, LS98, LZZ98, MP98, MSSF95, NBG93, PSK98, RB96, SD90,
SI93, SSF90, SMF91, VV96, VF92, VFM+90, WM93, BPS93, Bau90,
BKM97, GPK95, Jur96, KW91a, LKL+97, LMRL98, Luk94, MM97,
OL93b, RK97, WO97, WNW91, WJV+96, CLQS99, MLBD92, RTG98].
theories [HVM99, NS95]. Theory
[Dya98, Gar90, Ron90, TNKM91, Bec99b, Ber97b, Bec99, Che99, CH96b,
Cul92, FY98, FPC91, FUS+94, FSI95, GHWD99, GW98a, GW98b, GBW98,
GHT98, GW91, HT98a, HOL98, HS95, JU91, KO97, KOH98, Kl97,
KA96a, Ko99, LSCA98, LDG99, LKL+99, MTR95, MP90, Mor93, Ob98,
PS98, RTG98, SLPP97, SABA97, SC94, SLH96, SACK95, TAC98, Wib99,
Yar95, ZFY95, Zho93, ZL94, ZG92, Dav97, Ron92]. TheRate
[DBT98]. Thermal [Bal98, DBT98]. thermally [OS91, Vya97]. Thermodynamic
[CG94, KLV94, CKP96, HW97, LV90, MM91, RE99, AOY096]. thermolysin
[GBE92]. thiazole [KS91, SW93a]. thiocarbonyl [FTD92]. thiocarbonyls
[TDFdC91]. thiophosphoryl [Kat93]. Thioproline [MRG97]. third [BC90].
third-row [BC90]. those [PMHRG97]. Thoughts [Koh98]. threading
[HT99b]. Three
[JLW99, AMY98, CDR+95, CNS96, CF97a, FPC91, HKK+97, HO97,
HCCC99, JTM+95, KTN99, NL91, NBB+99, SLH96, YB95a]. three-
three-dimensional [CNS96, CF97a, KTN99, NL91, NBB99, YB95a]. three-electron [FPC91].
three-membered [AMY98, HKK97]. through-water [TRG99]. thymine [RTGJ98]. Ti [JFR92a]. TICT [GP94]. time [ACB92, BSS97, FHB99, GS93, GJD94, GT98, Kna92, KID93, LMB96, LCA94].
time-independent [ACB92]. time-scale [FHB99]. TIP3P [JJ98, SK95].

TIP4P [JJ98]. titanium [JB98]. TICT [GP94].


transforms [NVK97]. Transition [Jen94, AB98b, ABC99a, ABC99b, BSGB98, BC96, BCM99, Bo94, BC95, CH96a, GGH98, HM90, LJ92, LDJ92, MM93, MK97, MM95, PASF96, RCAA99, SH91, SB95, dVM91]. transitions [BK97b, MC99]. transport [AM99]. trapping [ISH98].

Treatment [JG93b, KN99, PPK92, TNS97b, BT96, FCNS98, GO95, PK95, TM93, TNS97a, VHV99]. treatments [HKG98]. tree [Cis93]. trees [BMP91, RWB91]. trehalose [DRF92]. trends [MK95, VRC91, VRC92].

trihalides [BT92]. trimer [KKE93]. trimers [GV94]. trimethoxyphenyl [WJ96].
trimethyl [Kat93]. trimethylphosphine [Kat93]. tripeptide [BH91b, HNH91]. triphenyl [IMP91]. triphosphate [Can93, HCC99].
triple [SMS98]. triplet [CLS97, FSC99, KHF91]. triquinacene [HIO93].

thiiricarbenium [GCC97]. trope [Pro93]. true [DKK93, DKK95].
truly [Ove91]. truncated [DZB94]. truncating [GK93]. trypsin [Kik96].

tryptophan [SU95]. tungsten [Van97]. tunneling [MGL99].


Two [HNS97, WCC91, AB97, ARL94, AD90, CW97, CCN90, CACD97, CBSR99, FD91, HBL98, HL96b, HYH94, HWH91, HT99b, Jia90, Jon91, KVK93, KTT94, KTH95, LTH96, MPJ98, MJPC98, SB98a, SSM96, YG92b].
two-body [MPJ98, MJPC98]. two-bond [Jai90]. two-center [Jon91].

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