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Title word cross-reference

(N – 1) [ACD+13a, ACD+13b]. (σ3, λ3) [TR12]. (σ3, λ3) [TR12]. +
[CXW14, GTK10, NMLD13]. 0 [UD12]. 1 [MG15, TS15b]. 1 – n [CYG+15].
10 [AC11b, TS15b], 13 [WYGW12]. 15 [AC11b], 17 [GZZ12]. 18 [LW16]. 2
[CWT+12, GSS13, MSBF16, MH10, SJD14, WvRSM14, YDL+10]. 20
[AC11b, LYL16, YVEI+17]. 24 [TS15b]. 3
[CM16, DVVP14, GMMH+16, GSS13, GPK12, LTT16, MG15, MA16,
MYT+14, PSS14, RVCFF13, TS15b, YLL11]. 4
[AFSW16, GWJJ12, ZTH+15]. 4d [Hil13]. 4f [Hua16]. 4 × 4 [SH14]. 5
[APY+16, LZH16, YLL11]. 512 [MKH15]. 6 [MCAY15, Rab12, TSQ12]. 62
[MKH15]. 63 [MKH15]. 64 [MKH15]. 8 [TN12]. 5 + 1 [YZL+15]. [n]
[uLhY11]. + [DDM+15, FD16, LCL+10, LdSRR16, LCWW10, RLA+11,
RRF11, SFBT17, UT14, YCGA10, YZ15b, ZCK+16, ZWY+10a]. +/+1
[TG12b]. + ⋄ π [CCCLCGRO14]. −
[CXW14, HBL12, JLH+14, LCWW10, RDT14, YCGA10, Yu12a, ZWY+10b].

[GT10].

[Ben17, KSK11, LGW12, LX11, LWD13, PTK11, Pie14].

[SKMS13].

[RDT14], {2} [RDT14].

[HAI+16].

[GTK10, LGW12].

[HAI+16].

[HA10].

[CM16].

[HJ13].

[SNKS10].
[DPSL16, GZZM16, LZL+15b]. \( \sigma \pi \) [CZY11, YWZ14]. Å1 Å' [MCLD10]. × [SRS14]. \( v = 0 \) [LWD13]. \( x = 1 \) [CWT+12, LZTV10].

- [CZY11, YWZ14]. ~A


-X [SZBM13]. -ZSM-5 [Pon10].

MgO [BS16b]. /MM [CZY11]. /TD [TS15b]. /Zn [GEP+14].


7 [ADF+10, MBR+15]. 7-azaindole [YYT12]. 7-tetraene [ABDGN12].

8 [AAC+16]. 8-formyl-7-hydroxycoumarin [LZHH11]. 8R [BG13].


= [CXS10, GPK+16, EPH+15, JLL+14, JJAB16, JJJ16, LDJ+10, LLL+11, LJJ+11, Li14a, Li14b, LGW12, LWW10, LWD13, MCK17a, MCK17b, PGS+15, PMG+16, Rab12, RDT14, SPS+12, SLIB12, TLdG+12, TFQ+11, TG12b, UT15, WWKS16, XiD15, YW12, YS13, YHCS11, ZYLL12, ZLLL12].

amino [CCCLCGRO14, CFC15, CB11d, FZL\(^+\)13, FP\(^+\)17b, GRL\(^+\)11, GRL\(^+\)12, HCP15, KLS10, KMLS10, LXL\(^+\)11, LP11b, MRO17, PHDH13, RSL16, SISK10, SZBM13, WC14, ZZWT12, ZKH\(^+\)10, ZHHX11]. amino-acid [KLS10, KMLS10]. aminoacid [MC10]. aminophenyl [LZL\(^+\)16]. aminophthalimide [WHL\(^+\)10]. aminopolycarboxylate [CMD13]. ammonia [BEPM14, CC12a, KT12, SNS16, SJZ\(^+\)15, VS14]. ammonia-borane [BEPM14]. AMOEBA [HLW\(^+\)17, MBE16, PZCL16, XP13]. among [KYB13, SH15, WGL\(^+\)11]. amorphous [Fom13]. amounts [FN12]. amounts [SFG\(^+\)17, FPV13]. amyloid [IO13b, LH11]. amyloid-beta [LH11]. analog [JBAM11]. analogs [DCHL12, LP11b, SISK10, VM11, WBT10]. analogue [PGW\(^+\)17]. analogues [LPS\(^+\)13, SGWA17, VVBL17, WS12, YLL11]. analyses [KASH14, KP11, PZBA13, SKGB13, VVJ15, XWW\(^+\)11]. Analysis [CDM\(^+\)15, HAI\(^+\)16, MOS12, AKMT11, AST\(^+\)16, ASL\(^+\)11, ARRCC15, Ano15-58, BK15, BH14, BSPP\(^+\)13, CAF\(^+\)13, CEBO15, CCC\(^+\)11, CAT\(^+\)13, CH14, DHF\(^+\)11, DJD12, DBK17, DCS15, EHSPT16, Fer17, FB12, FHW\(^+\)11, FHK\(^+\)12, GVP\(^+\)10, GLW13a, GLW13b, GND\(^+\)12, GCP\(^+\)13, Han11, HCD\(^+\)10, HPSK12, HHT\(^+\)13a, HHT\(^+\)13b, HDHL15a, HDHL15b, HDHL15c, HHWL17, Hug12, Jan16, JHH\(^+\)13, JJJ\(^+\)14, JZM14, JX10, KG13, KG\(^+\)Y15, LL13\(a\), LPS13, LMZ\(^+\)11b, LFM12, LAHS16, MDT13, MJ14, Mez10, MADWB11, MCLD10, MGS\(^+\)16, MCK17b, NIIT15, NS17, OXBW16, OC14, PTK11, PRT\(^+\)17, PTB\(^+\)15, PPUBGD10, PV12, PS14, RDT14, REL17, RL18, SYL\(^+\)10, SBB10, SFR\(^+\)11, SSS15, SMDK16, SS13c, SPR\(^+\)13, TYN15, TCB16, TD10, TT\(^+\)10, TS10b, UKS11, VBMA13, WNP\(^+\)16, Wei12a, Wei12b, XFG\(^+\)15, YK13, YNH\(^+\)17, Yes12]. analysis [Yes15, ZCS\(^+\)15, ZBB16, ZH12, vSGP10, ZSB\(^+\)11]. Analytic [MDTD13, SZX13a, SZX13b, MY17b]. Analytical [CCB15, HNWFO7, HNWFO12, LBGS16, SFG\(^+\)17, CHC\(^+\)13, FBY\(^+\)17, HH16a, KN17, KTSW11, MK13a, Pon11, ZWF15]. analytics [JZL\(^+\)17]. analyze [LP11c, OVPK15, QLQ11, RL18, YK011, dVAG16]. analyzer [JJW\(^+\)14, LC12, PVZ13]. Analyzing [BD11, MRB14, BCP\(^+\)10, LKS\(^+\)17, PHT17, SWA13, WES13]. anapole [ZPP\(^+\)16]. anatase [HRL11]. and [KB10, Pog10]. and/or [KB10, Pog10]. androstenedione [VCM15]. angle [CKP10, GBFD12, XML\(^+\)15]. angle-dependent [CKP10]. angles [BKLA13, EJ13, FZY\(^+\)12, GREA11, KTK17, LDH\(^+\)14, OZ14, YZ16]. angular [ENKK\(^+\)17]. anharmonic [Kow11, SSWX14]. anhydrase [SSP\(^+\)13]. anion [CG15, LC10, uLhY11, SDF12]. anionic [GZZ12, GWJ11, HPL13, JCP14, QZ10b, ZYR\(^+\)15]. anionic-water [JCP14]. anions [PVS12, RTD14, RJS17, ZYW\(^+\)10b, ZYL\(^+\)12]. anisotropic [Ano10a, CAT\(^+\)13, EPH\(^+\)13, ENKK\(^+\)17, NLP\(^+\)16, SLX\(^+\)15, SN10]. anisotropy [CP12, LPLB16, ZLZ14]. ANN [XWW\(^+\)11]. annealing [RHJ11, SHM11, SHL\(^+\)11, ZC14, LMZ11a]. annihilation [BL12]. Anomerization [SM17]. anomers [HH11]. ansatz [Bou14]. answer
Aromaticity
[CD16, AH10, AF16, Ano11, BY11, FC16, FNSF11, GRD10, HSB11, JHM10, KASH14, LZH16, MP11, YOP16, FB12].

arsenic/phosphorus [GWX12].

Artificial [CSAdOM17].


Atomic-resolution [BMFG16, NPG17]. Atomicistic [BH13, CHK10, MBA14, SE14, BLKP12, CZA11, DDP16, HDPM14, LZ12, MSC10, MMZ14, RO14b, RSG10, ZST14]. atoms [ARAG17, ARLP13, BSP13, DC13, EV14, GAM14, HSB11, HGCCGR16, IN13, LSH12, Mit13, Pyy13, SFCCK14, SFCCK15,
MC10, MA16, MS13, MPNS13, MMZW14, MFR+17, MO15, MNNK10b, NC12, NC13, NIX+10, NG10, OVPK15, OZLSBH12, PRP15, PC11].

**based** [PSC11, PBBP11, PN13, PKIC11, PPJ14, PLH16, PBE16, PPUBGD10, RLDJ17, RZG+13, RVP+11, SM14b, SFG+17, SLP+12, SLX+15, SFDE16, SLC+17, TYZ+16, Tak14, TTB+10, TS14, VGV+11, VVJ15, VKC10, VSA11, Vor10, WXL+12, WCDM11, Wei12b, WL14, WS13, WDHZ13, YJN+11, YZ16, YWJ+16, YZZ16, YDL+10, YJ11, YN15, YS13, YS15, YS10, YZZ+17, ZSLL17, Zha12b, Zha12a, ZY14, ZM10, ZYL+12, ZT14, dCLFGL13, dSVdM16, dVZ17, NKJ16]. **based-on** [CDS16].

**bases** [CWZB10, KASH14, MSLS10, SBW12, ZLL+10, Zha12a, ZBMZH15].

**Basic** [CMvG10].

**basin** [JLH+14, RDRC16].

**basin-hopping** [JLH+14].

**basins** [SBN13a, SBN13b].

**Basis** [BLF14, BRLS08, BRLS12, PHK14, SN16b, TKN13, ACD+13a, ACD+13b, BLFZ13, BLL13, BLBG+13, BS10a, BLG10, CC11, DBM+15, DLZ15, Fer13a, HSN14, Hll13, HBL12, KK17a, KNP+12, LBH+11, LCW12, Leh15, LYC+13, Mit13, OAN15a, PML+12, PGdO+16, POB13, Pla11, PD11, RLD12, SWM10, SGL10a, Sea10, SNKS10, Sun15, SG13, TH13, WX12, ZPP+16, ZLT13]. **Batch** [WHJH13, TJB12]. **bath** [CSEMB+16, MO15, Vor12, WAM17]. **BaTiO** [BE12, EB12, EBK13]. **Bay-type** [WvRSM14].

**Bayesian** [Fer17, GZ14, VZ14]. **BayesWHAM** [Fer17].

**BayesWHAM** [DZT11].

**Be** [LDJ+10, EPH+15, KV15b, LZW+11, NDG14, SMGB11, TH13, TCPPC14, Zha12b, BWKW10a, CCM15, CM16, ZLY+16]. **Becke** [FPV13].

**BeH** [ZLY+16, ZLY+16]. **behavior** [BVY+12, CME11, CSAOM17, FCD10, FTR15, KRTB10, LZY+12a, PD11, TLdG+12]. **belief** [GFPSD17].

**Benchmark** [WSZW15, AF14, ANH+11, cCVG+14, GAI14, KG15, RS13, ZWGO16, IKN13].

**Benchmarked** [XYW+14]. **Benchmarking** [Ben17, Hug12, LCM+14, GP11b, HRJ+14, HRJ+15, HZ13, JRSHP14, RSG14].

**benchmarkings** [GpdC+16]. **benchmarks** [ZDKM12]. **bending** [KB11c, Sch13]. **Bennett** [BB11b, KB11c, dRBO13].

**benzaldehyde** [Lu11].

**benzannulation** [YZL+15]. **benzene** [BPM15, BRLS08, BRLS12, CR14, Fom13, FTR15, FPRS14, SNS16, SGS+16, VVJ15, YHCS11].

**benzenesulfonamide** [SSP+13]. **benzenesulfonamides** [ALK+15].

**benzenesulfonyl** [YZGS14b]. **benzimidazole** [SJ16]. **benzo** [GKR13, Ray13, RKG11]. **benzo-** [GKR13, Ray13, RKG11]. **benzoquinones** [GNA+12].

**benzyl** [NDG14, YZGS14b]. **benzyne** [FC16]. **Bergman** [DHL12]. **Berne** [SLX+15]. **beryllium** [CME11, DLT17, Kop17a].

**Best** [KPF+15, AOW11, EK17, KM13, NG10]. **Best-First** [NG10]. **Beta** [KRSC12, HLH+12, Hug12, LH11, LJ+12, SKKS13]. **beta-barrel** [LJR+12].

**beta-complex** [SKKS13]. **Beta-decomposition** [KRSC12]. **beta-peptides** [HLH+12]. **Bethe** [KK17b].

**better** [AF14, BM12, KDS17, yOaCG10, XHL16]. **between** [ALW+10, ASL+11, AR10, ACS12, CCCLRO14, CZH12, CQFC10, COOH14, CB11a, DHF+11, Den12, FD14, FC16, GYX+10, GO13, Gav12, GKSS14].
DGH+11, EFAC13, EK17, EWK+13, EP12, EB12, EBK13, FAA15, FE14, GRARO+14, GMI16, HASR+12, HYL+11, HS14a, HB14, HSH15, Hel13, HG10, HG13, HBL12, HYUS11, JCG+11, KK17a, KB10, KKN11, KGK12, KRK+13, KERY+16, KCMPG12, KKL+13, KSH+17, LEEdldV17, LMZ11a, LCH10, Lyc+13, LCA17, LyG13b, LCM+14, Lun12, MCLD10, MCK17a, MCK17b, NWW17, OHNK11, OLA15, OOT15, OZLSBH12, PBLdS12, PTK11, PKH14, POB13, PBBP11, PDG+16, PN13, PGW+17, RAR+11, RHT+15, RLD12, RR11, REV+17, RI10, RK15, SH15, SRSLO15, SP13, SS16b, SCW11, SWPR11, SRS14, SDMS13, SHB17, SHTT11, TLdG+12, TS10a, UHH+11, VLb+10, VKAM12, VKNT16. calculations [VHR16, VFRAR16, VI17, WC13, WSZW15, WTH+16, WXY14, XYW+14, YWJ+16, YD17, YN15, ZRCC11, ZLT13, ZLZ14, ZWMW10, ZH12].
CASPT2 [SGWA17, VFRAR16]. Cassandra [SMRM+17]. 

change [EMD17], changes [GDV17, GBS+17, HB15, LK13, MJLV14b, MO17, RO14b, YZGS14b].

Changing [XVN17, LLvdG10]. channel [HYYZ13, PVL+13, SFJT17, SY16b, TCX+13]. channels [KC13a, LL10c, OKIS17]. character [BMB13, Cas14, RIJ+11, YSSB12]. characteristics [DPSL16, Gav12, LT14, Mat14, RDT14, TZ11]. Characterization [VT14, XWSW13, CBP+15, DGL+13, GBW+14, GZZ12, Kop15b, MJBMI2, MPA10, RNP13, ZYG+14]. Characterizing [LH11, PRSG13, She12, Yu12b].

charged [BK13, KD10, MRO17, NPP13, RJJS17, Tsi14].

MFM$^{+12}$, MFEM$^{16}$, MSÅK$^{12}$, PGCT$^{+12}$, SGM$^{+13}$, TKXT$^{13}$, XFG$^{+16}$, XLYZ$^{10}$, YKH$^{+10}$, ZSTI$^{14}$, ZPP$^{+16}$, ZYW$^{+16}$, ZZWX$^{11}$, All$^{11}$, ABB$^{+12}$, ABB$^{+13}$, BCJC$^{+14}$, BHI$^{13}$, CCCLRMO$^{14}$, CCJ$^{+11}$, DPOS$^{16}$, DZA$^{11}$, DHE$^{+12}$, FMSG$^{12}$, GS$^{14}$, GAI$^{13}$, GD$^{10}$, GHV$^{17}$, HCB$^{11}$, HS$^{16b}$, HDH$^{12}$, HZ$^{13}$, HV$^{16}$, IHH$^{15}$, KCI$^{13b}$, KG$^{11}$, KV$^{15b}$, LC$^{10}$, uLhY$^{11}$, MS$^{13}$, MS$^{16}$, ME$^{10}$, OSHG$^{17}$, PGC$^{12}$, PPUBGD$^{10}$, PVS$^{12}$, RCR$^{+16}$, Rez$^{16}$, RK$^{15}$, SLY$^{+10}$, SRR$^{16}$, SNS$^{16}$, SNGD$^{+16}$, SY$^{16a}$, Su$^{10}$, SDSMS$^{13}$, SDL$^{14}$, SIG$^{+11}$, SIG$^{+15}$, TF$^{15}$, TLA$^{10}$, TRA$^{+16}$, VZY$^{13}$, WXL$^{12}$, WCDM$^{11}$, WS$^{11}$, XWSW$^{13}$, YDX$^{16}$, ZCK$^{+16}$, dCLFGL$^{13}$, FHW$^{+11}$, Spr$^{10}$].

computationally [JJAB$^{+16}$]. computations [AGB$^{+13}$, B LBG$^{+13}$, CC$^{+12b}$, SRL$^{+15}$, VECT$^{12}$, VAMS$^{14}$, YB$^{16}$, dACP$^{+12}$].

compute [HDM$^{+15}$, KK$^{17a}$, YAS$^{13}$, dVAG$^{+16}$]. computed [CCYL$^{+11}$, Fra$^{15}$, Fra$^{16}$, HJ$^{+13}$, IIHY$^{15}$, RLDJ$^{+17}$, UKS$^{+11}$].

Computer [CLC$^{+11}$, BV$^{14}$, CBP$^{+14}$, DSK$^{17}$, GP$^{12}$, KSH$^{+17}$, SYN$^{+12}$]. Computerized [VBDS$^{+11}$]. computers [CSSB$^{+11}$, ESB$^{+13}$, TJB$^{+12}$]. Computing [Ano$^{+10a}$, GK$^{15a}$, HDL$^{+17}$, KHW$^{+17}$, PBDW$^{11}$, SN$^{10}$, ACD$^{+13a}$, ACD$^{+13b}$, BZB$^{+13}$, CHC$^{+13}$, CKKK$^{+16}$, GM$^{17}$, LPLA$^{+13}$, MKI$^{13a}$, MKO$^{+13}$, OV$^{14}$, OPB$^{+12}$, Rod$^{13}$, TF$^{15}$, XYX$^{17}$, Yan$^{14}$, ZWL$^{+13}$].

concatenated [PSP$^{+15}$]. concentrating [LLL$^{+10}$]. concentration [IPAA$^{+11}$].

concept [GRL$^{+11}$, GRL$^{+12}$, dSVdM$^{+16}$].

congestion [KNE$^{11a}$, XLYZ$^{10}$]. condensation [KNE$^{11a}$, XLYZ$^{10}$]. condensed [HRB$^{+17}$, RSLML$^{12}$, VKAM$^{12}$, dSdS$^{12a}$, dSdS$^{12b}$]. condition [IKN$^{+13}$, MTvG$^{+12}$].

conditional [BMPML$^{+13}$]. conditions [BRGN$^{+12}$, KB$^{14a}$, MO$^{+15}$, MO$^{+17}$, NO$^{+16}$, SIE$^{+15}$, SKMS$^{+13}$, TCPPC$^{+14}$, VECT$^{12}$].

Conductor [KB$^{14b}$, SDF$^{+17}$]. Conductor-like [KB$^{14b}$, SDF$^{+17}$]. conductors [MRB$^{+14}$, NFI$^{+16}$]. cone [BKLA$^{+13}$].

Configuration [SS$^{+13a}$, Cas$^{+13}$, CTP$^{+13}$, EK$^{+17}$, GA$^{+14}$, GP$^{11a}$, HBL$^{+12}$, LC$^{+10}$, MIS$^{+15}$, ZRCC$^{+11}$]. configurational [RO$^{+14a}$, WDHZ$^{+13}$].

Confining [NSP$^{+15}$, CDB$^{+10}$, FTR$^{+15}$, Vy$^{+15}$, Vy$^{+16}$]. confinement [TM$^{+16}$].

Confining [WRG$^{+17}$]. conformation [AST$^{+16}$, EJ$^{+13}$, PVJ$^{+10}$, SEF$^{+16}$]. conformational [SV$^{+11}$]. conformational [JJAB$^{+16}$]. conformational [JJAB$^{+16}$].
crystalline [DOM+11, DSLD13, DB12, EP12, EFOD13, GS12, DCOD13, RB13b, WDLG12].
crystallography [YW13], crystals [HZSS17, KGHC15, KLN12, KB16, LPS11, PLP+16, SFDE16, VECT12, You10].

CTOCD [PC14].
Cu [Rab12, RHT+15, TS15b, WRG+17, AMK11, CR14, ČMD13, GEP+14, HSH15, Mor15, PGS+15, PXXW10, PH12, RHT+15, SB10, WGN+16, WGLG+16, XP13, ZRCC11, ZSWL12].
Cu-O [ZRCC11].
Cu2II [WGLG+16].
Cuby [Rez16].
CuCN [TS15b].
CUDA [SR11].
CUDA-enabled [SR11].
CuE [TG12b].
curcumin [AMK11].
Curie [WMW11].
curing [LPMT17, PPH+14].
Current [NS17, ABM+15, FNSF+11, GWT+17, HLBLCCG15, PCLL11, PZM15, Vik11].
current-density [Vik11].
currents [RVB+12].
Curvature [LPLS16, RR12, NW17].
Curvature-dependent [LPLS16].
curves [BBI+11, LSH+11].
cut [DH14].
CVD [NIIT15].
CX [LGW12, EPH+15, ZYLL12].
CXH [CKL+11].
CXHM [LDJ+10].

cyanide [LZHH11, LLW12, TLY+12, VVBL17].
cyanide-chemosensing [LZHH11].
cyanides [PGS+15].
cyano [PKK17, TS10b].
cyanobacteria [RCM+13a, RML+15].
cyano [RCM+13a, RML+15].
cyanovirin [VM11].
cytochrome-P450-mediated [MRR11].
cytochromes [APA+14].
cytosine [JS17a, LZH+11, ZZY+16].
cyclizations [DCHL12].
cycloadditions [YZN13].
cyclobutadiene [SFM14, MCC11].
cyclized [QZ10a].
cyclodextrin [DBG11].
cycloguanil [APA+14].
cyclohexane [CROBY16, SNDK16, SAVG15].
cyclohexanes [SNDK16].
cycloocta [ABDGN12].
cycloocta-1 [ABDGN12].
cyclooctatetraene [DP11, SP13].
cyclopentadienes [LZH16].
cyclopropenylidene [VPV12].
cyclosporin [QZM11].
CYP11B2 [RVP+11].
CYP11B2-mediated [RVP+11].
CYP19A1 [VC15].
CYP2A6 [ALW+10].
cysteine [CPK12, SDL14].
cytochrome [EH13, BS16a, MRR11, SL+10, SOYC12, TN10, TDP+12, VCM15].
cytochrome-P450-mediated [MRR11].
cytochromes [APA+14].
cytosine [JS17a, LZH+11, ZZY+16].
detonation [LWWG12]. developers [GKV+13]. Developing [CK17, DSK17, LPS+13]. Development [GLB16, GMMH+16, LLJ12, MMB+17, MMZW14, RZG+13, RLD12, TNYN16, WPM+15, ZA15, CYG+15, GMASBF16, GCP+13, LPLA13, PZA15, PPM15, WDHZ13, YWZ14, ZsA10, ZSYH12, CRC13, VKC10, WCDM11]. developments [YWJ+16]. Deviation [CSAdOM17]. deviations [HDL+14, KG15]. devices [DJX+11b, DJX+11a]. Dewar [Bac12]. DFT [SIG+15, YJ17, ZZY+16, AALCM11, AR10, AF14, ASMS10, BTMS12, BIL10, BTB+11, CCB15, CH10, cCVG+14, CXS10, DJD12, EFAC13, FVP14, FPRS14, GMASBF16, HSH15, HRJ+14, HRJ+15, HBI+17, JRSHP14, KG15, Kar17, KT12, KKL+13, KM13, KP10, LEdOLdlV17, LRRB12, LZZ+10, LZHH11, LZX+10, LSH+11, LYSS11, LZLC13, LH14a, LLSW14, LCM+14, MMS16, MTD16, MG15, Mat10, MS11, MVK10, Mor15, MCK17a, MCK17b, NKJ16, NMLD13, PTK11, PHK14, QLYL10, RDF+11, RS14, RRC+15, RN17, REL17, RKB+14, RK15, SRF+17, SWM10, SRL+15, SDL14, TG12b, Ts14, Ts15b, Ts17, VVJ15, VECT12, VAMS14, WKL12, WYGW12, YZGS14a, YSRS10, YZ15b, ZCK+16, ZWGO16, ZZWT12, dSDdAR10].

DFT-based [NKJ16, NC12]. DFT-derived [REL17].


DFT-based [NKJ16, NC12]. DFT-derived [REL17].


diagonization [BK9+11, HKR+14]. diagonalization-free [BK9+11, HKR+14].

diagonization [OV14, VED10, ZY14]. diagrammatic [WWD14, YD17].

diagonization [OV14, VED10, ZY14]. diagrammatic [WWD14, YD17].

diagonization [OV14, VED10, ZY14]. diagrammatic [WWD14, YD17].

DFT-based [NKJ16, NC12]. DFT-derived [REL17].


diagonization [BK9+11, HKR+14]. diagonalization-free [BK9+11, HKR+14].

diagonization [OV14, VED10, ZY14]. diagrammatic [WWD14, YD17].

diagonization-free [BK9+11, HKR+14].

DFT-based [NKJ16, NC12]. DFT-derived [REL17].


diagonization [BK9+11, HKR+14]. diagonalization-free [BK9+11, HKR+14].

diagonization [OV14, VED10, ZY14]. diagrammatic [WWD14, YD17].

diagonization-free [BK9+11, HKR+14].

DFT-based [NKJ16, NC12]. DFT-derived [REL17].


diagonization [BK9+11, HKR+14]. diagonalization-free [BK9+11, HKR+14].

diagonization [OV14, VED10, ZY14]. diagrammatic [WWD14, YD17].

diagonization-free [BK9+11, HKR+14].
distance-dependent KCPMG12, distances BLDK+13, SSWX14, SMGB11, distinction ZY14, Distinguishing FD14, GMBX+16, Distributed XFG+16, BMBJ11, UIW+10, XFG+15, distribution [Bou14, HDK+12, HNS16, JLCA17, SYH12, TKN10, YKO+11], distributions [AS15b, BCSCJ+13, GWF11, GMG+10, LRER13, disulfide ZYS+10, ditetrazoles ZZWX11, dithiolate GS11, dithiolene KTK17, Divalent WC14, BMB13, divergence PNG10, diverse LLC+10, diversity WF16, Divide NNK+16, BRP+12, BGR13, BK17b, KKKN11, WX12, YN15, Divide-and-conquer NNK+16, BRP+12, BGR13, KKKN11, WX12, YN15, divide-expand-consolidate BK17b, Dividing SLT+15, DLPNO [CSGOA17], DLPNO-CCSD [CSGOA17], DMF [YZL+15], DMPC [GBL+11, PS10, SLX+15], DMS [RAGLI1], DNA [AB10, DNN15, BD11, BH13, BZH14, DMN14, FPB12, GWX+12, HKD+12, HQC16, HvM12, IPAA11, KvdV14, IW11, LMZ+11b, LIT12, OHNK11, OLA15, QLQ11, SM14b, She12, SM15, SM16b, SZSZ16, YZWC11, YJXZ13, YS10, ZLL+10, DNA-backbone [AB10], DNA MR [SR11], DOCK [ABM+15, BS10c], docking [ABM+15, BMR11, BAMR13, BBOB16, BBP11, BCG10, BEL+11, CSSB11, DFF+15, DSX+11, ESB13, FM10, FTW12, FRLN10, GLB16, GSHM10, GPS10, GZM11, HDM+15, HHLW11, HZ13, KERY+16, Kri10, LS11a, LLC+10, LL10b, LLL+13, LJL+11, MMM+16, MPNS13, MP11, MFR10, NMF+14, NHK+13, NG10, OCLM14, OZS+13, PLAG11, PLV+11, Pro16, RMP+13, SA13, SHL+11, SKKS13, TO10, VSD10, Vor10, WdVN12, WZ17, XML+15, ZL11, ZW13, ZSB+16, dVZ17, docking* LZ11, docking-rescoring [BMR11], DockoMatic [JBAM11], Does [MBFG15, MIS+15, SV15], DOI [Ano15-59], Domain [KNE11a, AC11a, IMK+16, MBT14, RJ16, SBFT17], domains [FCPMJ14, OOK11], dominant [Hua16], donor DGL+13, Gil11, Lu11, MSV16, MIS+15, donor- [MIS+15], donors [LC10, TZ12], dopant [SRL+15], doped [GAMAC+14, LLC17, PGC12, TN12, VS14, WMW11], doping [HYL+11, LLD17, WMW11], DOT2 [RTP+13], dots [DPAB16], double [Alg17, BE14, CCB15, CGR16, CC11, FC16, KM13, LBH+11, LYG+13, LLL+12, SGPS+17, SP13, Sea10, YYT12, ZLY+16], double-Hybrid [CGR16, LBH+11, SGPS+17, Sea10], double-wall [BE14], doubly [SZX13a, SZX13b, ZWIX11], Douglas [YS13], DOX [RCP+16], DPO [WGL+11], DPPC [LBDP12, rWGS17], DPT [BH13, BZH14], Dramatic [MLY+13], Draw [LBB+15], drawback [BRGN12], Drew [IPAA11], driven [BLSL11, DSM+11, HXM+16, KC13b, LLL+13, LLL+12, REL17], driving [RN17, YZ17], Drude [LKVdSM15, Ric16, SM14b, ZM10], Drug [GSHM10, MBA14, FLM11, GMASBF16, Ibr11, ISP+10, PC11, PVJ10, VHA+10], drug-like [VHA+10], druggability [LG14], drugs [PPUBGD10], DSCs [YI11], DSPMP [FZL+15], DsRed.M1 [SGDT10], DSS [GZM11].
DTTO [MCAG+16]. dual [JCG+10, MA16, TMJ15]. Duncanson [Bac12].
duplex [HDK+12]. Durandal [BSZ+12]. during
[GNDA+12, LBC+12, MJLV14a, MJLV14b, PNG10, RSKG14, dCDP15].
dyad [KP10]. dyads [KCK+15]. dye
[ACS12, JYS+12, LSL+12, YJN+11]. dye-aggregates [SLP+12].

dye-sensitized [ACS12, JYS+12, LSL+12, YJN+11]. dye-sensitizer
[YJN+11]. dyes [DBM+17, VAA14, WJG+13, YJN+11].
dynamic [LKL10, TNYN16, AKK+16, BS10a, BMB13, CVT+11, ESM+12, GBL+11, 
Hel13, MB14, NYN17, OPR16, Vor12, PBDW11]. dynamical
[ALH+10, EFOD13, Ham11, VPR10]. dynamically [HS17].
Dynamics
[CPV+12, LK13, MFEM16, AALCM11, AG11, AS15a, Aki16, ASL+11, 
ABD11, APK14, AB16a, ALH+10, BHB12, BSL11, BDTP11, BJSI12, BW15, 
DMN15, BMBJ11, Bow16, BEL+11, CTR13, CS14, CH16, CCOH14, 
CCW+10, CHKR10, DASA15, DGH+11, DSD+11, DZH11, DLZ15, EP10, 
EK15, ETLS17, EFOD13, Fom13, FBM11, GBL+11, GDV17, GR11, 
GWZ15, GCW14, GGM+12, GP11b, GC11, HZ11, HCD+10, HP10b, HPSK12, 
HJ10, HHWL17, HRD16, HC14, IUK+11, ISK14, II10, IPAA11, JIS13, JA10, 
JBSQG11, JCG+10, JAH+10, JST10, JMS14, JS17b, KCK+15, KV+10, 
KUDG12, KGHC15, KDB13, KB14a, KNE11a, KERY+16, KLOS10, KSR+16, 
KG13, KV15a, KVR10, LL12, Lar12, LWK+14, LH11, LJR+12, LL13a, 
LRvdSM15, LCH10, LSY+13, LMI14, LPE+10, LLTC12, LZS+17, LPLB16, 
LLT2, LBDP12, MBT14, MKS+12, MSC+10, MJ14, MN15]. dynamics
[MCRL17, MFEM15, MADWB11, MKM+17, MB16, MHR11, MO17, 
MIOM13, NPTS16, NST14, NFDP13, NFG+13, NNK+16, NHK+13, 
NTY15, Oht16, ON14, OGL10, OCL11, OLY17, OT12, OCW+15, PMC+17, 
PSS14, PAK15, PH17, PL14, PM13, PD12, PHT17, PVZ13, PS10, PVAM16, 
RS12, Ras17, RO14a, RO14b, RFN15, RR14, RdA12, RVdB16, RLG14, 
REL+14, RSR15, RSB+13, SHMO11, SL+15, SWM10, SSWX14, SOM+13, 
SJ17, SYN+12, SM16b, SK13, SKMS13, SLL13, SJ16, SV11, SBvG14, 
SAvG15, Tac17, TNYN16, US11, Vor10, VM11, WKLC12, WBN+13, 
WAM17, WC11, WHL+10, WH11, WWKS11, WLC2, WES13, WG14, Wu10, 
WBVE16, YPvD13, YJXZ13, Yon16, Yu12a, ZZY+16, ZX11, ZDKM12, 
ZBP11, ZP13, dCLFG13, dSVdM+16]. dynamics-based [Vor10].
DynamO [BSL11].

[Ano11, JHMB+09, JHMB+11, WD10]. easy [TKT11, VVV+15b, Yes12].
Ebola [OLY17]. economic [PN13]. Ecoupling [dVAG16]. edge
[DJX+11b, PDG+16]. edge-modified [DJX+11b]. editing [You10]. Editor
[GKR13, GPGSM12, JW12, Ray13, RSLML12, WM12, dSDs12b, vLBBR12, 
Lli12, BCJC+14, KRC14, Man13, VVB13]. Editorial
[Ano16-56, Ano16-103, Ano16-104, Ano16-105, Ano16-106, Ano16-107, Yan16, 
Ano16-129, Ano16-108, Ano16-109, Ano16-110, Ano16-130, Ano16-111, 
Ano16-112, Ano16-113, Ano16-114]. Editorials [BEFS13]. Effect
[HDL^{+17}, SL10]. ended [RJR14, Zim15]. endo [FB14a]. endohedral [FL15, GLF16, MCK17a, MCK17b, ZSL^{+11}, ZYG^{+14}]. endohedrally [DM15, VIT^{+15}]. endothelial [JAH^{+17}]. endpoint [BB11a]. ene [GRCL12, FB12]. enediene [DCHL12]. Energetic [JW12, CG15, MCAG^{+16}, SLHW09, TPL^{+10}, YSRS10, ZZWX11, ZYL^{+12}]. Energetics [SFM14, BK17a, BMFG16, DSF17, JJH^{+13}, KB13, MP13, MBRC16, OCW^{+15}, SJ11, SNS16, SDB^{+16}, ST13, SFBT17]. energies [AF14, AS14, AG12, BW11a, BLF14, BVHI17, BS16b, BE16, CHG^{+16}, CMD13, CH10, CTP13, CBG16, DHOG13, DHF^{+11}, DPOS16, FGM11, Gil11, GP11a, Gri3, HAGK10, HH10, HH11, HLW^{+17}, HHWL17, IKN13, KSH13, Kar17, KJDB12, KB11b, KPY13, LW11, LHWH14, LH14a, MCS11, MS13, MSAK12, MBE16, MMJ10, NWW17, NMF^{+14}, OBW12, yOTn16, OAN15a, OSR16, PGCT^{+12}, PPJ14, RLKD17, RDDS10, RAR^{+11}, RO14b, RZ16, RR14, Rob13, RJS17, SRR16, SK12, SRL^{+13}, SOD^{+11}, STM^{+15}, SGWA17, TSI14, TSN16, UD12, VVG13, VECT12, VM11, WBT10, WS10, WJG^{+13}, WG12, WX12, YAS13, YMP14, ZZ14, dALdS^{+15}, dRBO13]. Energy [DK11, GS16, IIHY15, JCGVPHT17, LFN^{+10}, LPLB16, SN16b, SSGS15, SKGB13, WM12, AMGB10, AC11a, A-Nao10a, AK10, ANKN16, BCSCJ^{+13}, BPM15, BRE16, BH15, BS16a, BRLS08, BRLS12, BACSCJ^{+10}, Bou14, BD11, BWMSM10, BB11b, BB11c, BG12, CM13a, CK10, CDM^{+15}, CLA16, CY09, CX10, CY11, CI13, CH16, CS17, CHR^{+12b}, CHR^{+12a}, CKP10, CMvG10, CPK12, CWZB10, DGH^{+11}, DBG11, DS12b, DH14, DWC17, EV14, FMNC11, Fer17, FCOGM12, FSSW17, FCCP17, FLM11, GS14, GS15, GHH12, GO13, GNO16, HDL^{+17}, He13, HDM^{+15}, HH15, HG13, HYMZ16, HYUS11, HJKJ13, HYD10, HDH15a, HDHi15b, HDHL15c, IMK^{+16}, ISN13, JCP11, JMLL13, JZ12, JZZM14, JX10, KCB^{+12}, KTT16, KB10, KNHN16, KN17, KHWB17, KB11a, Kop15a, Kop16, Kop17a, Kop17b, KLS10, KMLS10, KCL^{+14}, LMZ11a, LZZ14]. Energy-adjusted [HH15]. enforced [BW11b]. engine [BEFS13, HC14, DBDP16]. enhance [EFH^{+15}, LZZ^{+15}, MIS^{+15}]. Enhanced [CFC15, HTS15, IMK^{+16}, KvdV14, BND14, KKO^{+16}, LC16, MBFG15, SL11, ZLT^{+15}]. enhancement [LLL^{+11}, MA17]. enhancements [Abr11]. enol [FD14]. enoyl [STM^{+15}, SJ16]. enoyl-ACP
Ensemble [PKIC11, MKM+17, YHH+13, ZWP11].

Ensembles [CDM+15, GO13, Gri13, PBDW11, PKIC11, RLDJ17, RO14a].

Entatic [HBR17].

Enthalpies [cCVG+14, HDK+12, LLH11, LWL+10, MRR11, WKC11, WDW12, ZWLX11].

Enthalpy [UCFR16, vADC+14].

Entropy [CHR+12b, CHR+12a, Pro16].

Environments [CCW+10, CB11a, JWST10, KKR+13, Lar12, LvG13b, LLT12, TLY+12].

Environment [JBSQG11, PAT+10].

Epimeric [HH11].

Epitope [CGBK13].

Epitopes [GRP+12].

Epoxidation [WCDM11].

Epoxides [BCP+10].

Equation [BCCO10, CD16, CLA16, Fer13b, Fer13a, FCE15, Fra15, Fra16, KK17b, RLS13, SK15a, SM16a, SG10a, WBVE16, XX17].

Equations [BYE+16, ZR10].

Equilibrated [WHAS+10, WHAS+16].

Equilibrating [OPR16].

Equilibration [LBDP12, SMP17].

Equilibrium [DSD+11, FD14, LLvG10, LvG13a, MCLD10, NHH16, SJWE10, WXY14].

Eric [Sch10].

ERKALE [LHS12].

Ermod [SM14a].

Errata [CHR+12b, HRJ+15].

Erratum [ACD+13a, Ano15-59, Ano15-58, Ano17z, ABB+13, BRLS12, CY13, Fra16, GLW13a, HNWF12, HvM17, HDHL15a, HDHL15b, ICS+13, JHMB+11, Li14a, MSK+12, RK16a, SFCCK+15, SB13b, SSM15a, WHAS+16].

Error [HAGK10, Hua16, PHK14, PB11, WNP+16, ZH12].

Errors [LEdOLdlV17].

ESCF [vW11].

Esculetin [LYSS11].

ESES [LWZ+17].

Essentials [DASA15, SKMS13, XTY+14].

Establishing [ZKH+10].

Estrone [AGM+13].

Estimates [GS16, GS15, NFG+13].

Estimating [RF15, KB11b, TTB+11].

Estimation [RLDJ17, BPE16, CZY11, Fer17, GLM+17, HHWL17, Hug14, JKS+16, MSV16, MRR11, OZS+13, PHK14, SY11, YOMT14, ZH12].

Estimator [FCPMJ14, WBF17].

Ethan [Tak11, ZLT13].

Ethanol [AAMD+11].

Ethylene [HLB15, WLC12].

Ethers [KGR13, Ray13, RKG11].

Etoh [KCS12].

ETS [CSM16].

ETS-NOVC [CSM16].

Eulerian [LWZ+17].

Evaluating [BY11, KPL13].

Evaluate [BY11, KPL13].

Evaluating [SJ16, WG12, HLS12, VL17a, XSZL11].

Evaluation [AYYO17, CHR+12b, CHR+12a, EP12, HG10, LLC+10, MBE16, MCK17a, RRRH12, RB13b, WM17, YD17, BMR11, BLF13, BLF14, DLT17, DS12b, GS11, HBI+17, ISO+13, KLOS10, Kos16, KSC16, LJW11a, LW11, LHHW14].
explosive \textsuperscript{YP\textsuperscript{+10}}. Exponential \textsuperscript{BBOB16, BB11b}. expressions \textsuperscript{Gav12}. extended \textsuperscript{GWZX12, KUDG12, LRvdSM15, SSWX14, TSN17, YB16, Pon11}. Extending \textsuperscript{LMZ11a, Man13, VBV13a, VBV13, PHH\textsuperscript{+12}}. extensible \textsuperscript{GWZX12, KUDG12, LRvdSM15, SSWX14, TSN17, YB16, Pon11}. Extensive \textsuperscript{LMZ11a, Man13, VBV13a, VVB13, PHH\textsuperscript{+12}}. external \textsuperscript{GCW14, JYC\textsuperscript{+16}, LAS\textsuperscript{+14}}. \textbf{Extension} \textsuperscript{HSN14, PFVL14, SDZ17, YHVM12, Cam15, LL11, RLLHL12, Ras17}. Extensive \textsuperscript{JW12, SLHW09, YB11, CF14, KM13}. extrapolation \textsuperscript{CC11, LYC\textsuperscript{+13}, OAN15a, SRR16}. Extreme \textsuperscript{HRHI17, Cam15, DS12a, JBSQG11}. Extremely \textsuperscript{ZM11}. F \textsuperscript{CXW14, CXS10, GPK\textsuperscript{+16}, GTK10, HBL12, LZJ\textsuperscript{+11}, Li14a, Li14b, PMG\textsuperscript{+16}, Rab12, STM\textsuperscript{+15}, TFQ\textsuperscript{+10}, TFQ\textsuperscript{+11}, TCPPC14, WLW\textsuperscript{+10}, WCY\textsuperscript{+11}, YS13, ZYLL12, ZLLL12, BWKW10b, CCM15, Chn10, H10, LZL\textsuperscript{+15b}, MLGB16, SYH12, TCPPC14, Yu12a, ZWY\textsuperscript{+10b}}. F-ATP \textsuperscript{SYH12}. F\textsuperscript{12} \textsuperscript{BBG\textsuperscript{+11}}. F\textsuperscript{12a} \textsuperscript{MLCD11}. F\textsuperscript{130L} \textsuperscript{ZJZM13}. FabI \textsuperscript{STM\textsuperscript{+15}, SJ16}. face \textsuperscript{GY10, Zha11}. Face-to-face \textsuperscript{Zha11}. faces \textsuperscript{PRJ\textsuperscript{+17}}. facilitate \textsuperscript{MDTD16}. facilitate \textsuperscript{HNTS15}. Facilitating \textsuperscript{CVG14, VVG13}. facilify \textsuperscript{ZM11}. F-ATP \textsuperscript{SYH12}. F\textsuperscript{12} \textsuperscript{BBG\textsuperscript{+11}}. F\textsuperscript{12a} \textsuperscript{MLCD11}. F\textsuperscript{130L} \textsuperscript{ZJZM13}. FabI \textsuperscript{STM\textsuperscript{+15}, SJ16}. face \textsuperscript{GY10, Zha11}. Face-to-face \textsuperscript{Zha11}. Facilitating \textsuperscript{ESB13}. facilitator \textsuperscript{Mez10}. facilities \textsuperscript{GP11b}. Facing \textsuperscript{SLT14}. factor \textsuperscript{WLF11, WC11, XMSZ16}. factors \textsuperscript{VKAM12}. Factors \textsuperscript{GMSV14, EFOD13, LBH\textsuperscript{+11}, LCW12, Pie14, VSA11}. fail \textsuperscript{WCWV15}. failure \textsuperscript{JWO15}. FALDI \textsuperscript{dLC17}. family \textsuperscript{PHC13, ZLZ14}. FAMSEC \textsuperscript{CSM16}. farming \textsuperscript{HPSK12}. Farm \textsuperscript{AGR11b, BSZ\textsuperscript{+12}, GZM11, HKR12, Kne11b, KDT\textsuperscript{+12}, LAT10, LAT11, NHH16, PPJ14, RB13a, RDDS10, SM14a, SR11, TRA\textsuperscript{+16}, VGV\textsuperscript{+11}, XSZL11, YZZ16, Yes12, dVZ17, DZA11, FGM11, GBFD12, Kan15, LFB14, LBG16, MDT10, MS12, MPBJ11, OV14, dRL11, Sch12, TJB12, Yes15, ZSS\textsuperscript{+13}, ZCM11, dSAdSL13, YWJ\textsuperscript{+16}}. faster \textsuperscript{HC14, AM10}. fate \textsuperscript{SIG\textsuperscript{+11}}. fathead \textsuperscript{TTL\textsuperscript{+12}}. FAU \textsuperscript{LZTV10}. FE \textsuperscript{JJAB16, BTMS12, LLLM11, LLSW14, VED10, WWKS16, Bac12, DAdGR15, GBGR16, PCH13, SSX\textsuperscript{+14}, YPd13, vADC\textsuperscript{+14}}. feasible \textsuperscript{VAMS14}. feature \textsuperscript{TD10, YS\textsuperscript{+10}}. Features \textsuperscript{FHMB15, ALW\textsuperscript{+10}, AS11, ABM\textsuperscript{+15}, DLW\textsuperscript{+10}, PLP\textsuperscript{+16}, WC11}. featuring \textsuperscript{Alg17, ZYW\textsuperscript{+16}}. feedback \textsuperscript{VHR16}. FeFe \textsuperscript{GS11}. Fehlberg \textsuperscript{AMGB10}. FeO \textsuperscript{TLY\textsuperscript{+12}}. FeP1d \textsuperscript{BK15}. FEBERUS \textsuperscript{DBDP16}. ferromagnetism \textsuperscript{HYL\textsuperscript{+11}}. ferromagnets \textsuperscript{ZA15}. FeS \textsuperscript{TLY\textsuperscript{+12}}. Festschrift \textsuperscript{HIS17}. FEW \textsuperscript{HG13}. FF \textsuperscript{LGW12}. FFLUX \textsuperscript{FP17a, FP17b}. FFT \textsuperscript{MYT\textsuperscript{+14}, WS13}. field \textsuperscript{AJR16, ALH\textsuperscript{+10}, BK\textsuperscript{S\textsuperscript{+11}, BCSCJ\textsuperscript{+13}, BCJC\textsuperscript{+14}, BY11, BW15, CRC13, CIK13, CYG\textsuperscript{+15}, CZA17, CLC11, CB11b, CB11c, CK17, DPNM11, DGPM14, DFF\textsuperscript{+15}, DMAH15, DP15, DGB\textsuperscript{+13}, DLZ15, EPD\textsuperscript{+11}, Gar12, GSD10, GZM11, HH11, HKR12, HLH\textsuperscript{+12}, HKR\textsuperscript{+14}, HM13, HJLV16, HCP15, ISO\textsuperscript{+13}, IHJ\textsuperscript{+13}, JSXH16, KLJ\textsuperscript{+17}, KSK11, KT10, KMLS10, KR10, Lar11, LvDH13, LC17, LPS\textsuperscript{+13}, LPE\textsuperscript{+10}, LN15, LLvG10, LvG13c, LL13b, LDG\textsuperscript{+15}, MRO17, MBC11, MCB\textsuperscript{+13}, MS\textsuperscript{+13}, MTvG12, MBE16
MLC13, MHRR11, MP17, NTNY15, ON14, PHC13, PG15, PZCL16, PLH16, PVM10, PS10, PNG10, Rod13, SH15, ST11, SM14b, SK17, SZBM13, Sie15, SS13c, SCSW13, SM15, SYZ + 17, SBvG14, Tak14, TYN15, VHA + 10, VPR10, VikI1, VVLG17, WXL17, WTH + 16, WC14, WZK + 13, WDHZ13, XP13, XVA + 16, Yan11, YWZ14, YJXZ13, YJ11, YN15, YCK16, YHVM12, ZSLL17.


First-Principles [CCJC10, DBM + 15, ELI2, EBK13, JCG + 11, LLLM11, LLB + 12, LCWW10, RRK16, TKN13, YPvD13, YRI3, wZbZ11, BPE16, BCCO10, BEL + 11, EDM17, GD10, GA14, LL10c, Lu11, MCF10, NNS15, RZG + 13, SK12, TKC + 11, TZ11, WXS + 12, WYL + 15, WD10, WZK + 13, YHCS11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC + 14, HYL + 11].


flexible-boundary [PL14]. flip [ZLHH14]. FLOODing [HNTS15, HNS16].


fluorescence [CH10, EJ13, ZLL + 10]. fluorescent [LZL + 10, NOS + 14, PGW + 17, WJG + 13]. fluoride [LZL + 10, MBRC16, NC12, Rab12, SRL + 15]. fluorides [Sán17].

fluorobenzene [KS13b]. Fluorophilic [vRWGS17]. fluoroquinolones
BZB+13, BG13, CHG+16, CR14, CWWH11, CSKH15, CSKH16, CC11, CNK97, CPLL11, CB11d, FD16, GA14, GHL17, GZL+12, GNCA10, GSS13, GEG11, GWPJ11, Han11, HDL+17, HNWF07, HNWF12, HG10, HZS17, IKN13, JCP14, JLH+14, JW16, JYS+12, KD10, KKPT11, KOP+14, KGHK12, KB13, KZZ+16, KLN12, LCW12, LBS16, LGW12, LBTV11, LBT12, LHKS12, LH14b, LLH17, LPMT17, MAK+14, MWJ+11, MFR+17, Mor15, MMJ10, NF17, NO16, NDK+16, Oht16, ORZ11, OM12, PAK17, PPH+14, Pie14, PD11, QZ10b, RJPB12, RS13, RB12, RSLML12, RHPWS13, RHT+15, Rui11, SPS+12, SH15, SFG+17, SCW11, SBT17, SEF+16, SE14, SH14, STS13, SMM15a, SMM15b, SKTT11, SZZS16, STS15, TLDG+12, TG12a, TS10b, VV14, Vik11. functional [VL17a, VI17, VLGK17, VED10, WKC10a, WHL10, WDLG12, WYT17, WHX+10, WL14, WTH+16, WGN+16, XYW+14, YJ11, YLZ+10, YS13, ZXS+10, ZWLX11, ZSWL12, ZLY+14, ZYW+10, ZLY+10a, ZLHH14, ZGS+10, dSdS12b, functional basis [PD11]. functionalities [KAG+12]. functionalized [KYKR15, LDSSR16]. functionalities [Ben17, CCB15, CGR16, DH17, DOM+11, DWC17, FPR14, HG10, HBI+17, KB10, KSH13, KSSH13, Kar17, KM13, LBH+11, LH14a, LKI6a, PW12, RSG14, Rui11, SGPJS+17, Sea10, SDM+16, SPR+13, SZX13a, VLGK+17, Yu12b, ZTH+15]. functions [BLZ+13, CD13, CC11, CVG14, Fer13b, Fer13a, FFA14, Fra15, Fra16, GSHM10, GZ14, KK17a, LRER13, MY17b, Mit13, MLCD11, PHT17, Pro16, RHRCH16, SPM14, SYDS11, Sun15, TNYN16, WZ17, TK13]. fundamental [CD16, XLYZ10]. furanosides [KRTB10]. Further [RTS+13, FVB10, PZA15]. fused [CZY11]. fusion [OLY17]. Fuzzy [FPV13, SK12, SK17]. fuzzy-border [SK12, SK17]. FXeOXeF [ARLP13].


Gas-phase
Generalized
[GH16b, KCPMG12, AB16b, BSPP+13, DSF17, FCE15, GH16a, LL10a, MA16, PS13, SZTSM10, SSBW14, WWKS11, WHM10, WBVE16]. generate [MPA12]. generated [HWLW11].

Geometrically [RIJ11]. geometries
[Alg17, HCP15, SRA17, Tak10, LXZ+10]. Geometry
gibberellin [HYYZ13]. gibberellin-binding [HYYZ13]. Gini [WF16].


Gradient [DS15, CDM10, HHHY10, KN17, SH15]. gradient-directed
Gradients [GP11a, WM12, BWMSM10, CCB15, HH16a, LBGS16, LFN+10, RSG14, SFG+17, SSWM09, SLG15, vLBBR12]. grafting [KKR+13].

gradient [GP11a, WM12, BWMSM10, CCB15, HH16a, LBGS16, LFN+10, RSG14, SFG+17, SSWM09, SLG15, vLBBR12].

grained [BLKP12, CAD16, HHWL17, JC16, KVQC+11, KLS10, KMLS10, LZ12, LZX16, LZZ14, LZLMP16, MLS10, MBC11, MBC13, NST14, RSG+10, SLX+15, SDZ17, SJ17, SM15, SA+G15, WBF17].

graining [BJP15, GMPB12, ML14].

gran [HLvdV13, PHH+12].

grand-canonical [PHH+12].

Grante [HLvdV13, PHH+12].

graph [WSH10, DH14, GPGSM11, GPGSM12, Ihli12, MCC12, PsdPE+10, Pog10, RNP10]. graph-based [DH14].

Graph [WSH10, PsdPE+10, Pog10].

Graph-theoretical [WSH10, PsdPE+10, Pog10].

Graphane [YZZ+17].

Gratzel [VAA14].

gravitational [DS15].

Grcarma [KG13].

Green [LWL+11, NSO+14, PGW+17, yOTn16].

Gregori [Ihl12].

Gregori-Puigjané [Ihl12].

ggreg [Ihl12].

Gregori [Ihl12].

Gregori-Puigjané [Ihl12].

Grid [BAMR13, HEMCZE+14, KP11, LZ11, LLZA12, MM+16, RLLHL12, dVZ17, CM13b]. Grid-based [BAMR13, HEMCZE+14, KP11, LZ11, LLZA12, MM+16]. grids [DH17].

Gro2mat [DK14].

GROMACS [AG11, Abr11, Gar12, GP11b, KPF+15, LRvdSM15, PHH+12, TKT11, KWG15, DDK14].

GROMOS [HH11, HLL+12, KAG+12, LGL11, LVG13c, MRO17, MSvG12, PLH16, PFV14, SBV10].

GromPy [PHH+12]. ground [BBI+11, CCM15, FAA15, GCM15, HH16a, Kop15a, LLBO12, LYC+13, LX11, LS11b]. ground-state [HH16a, Kop15a, LLBO12].

group [Kan15, KV15b, LPS12, TN10, WGL+11]. growing [JZ17, Zim15].

growth [FCL+10, LL10, LZLMP16, MZZ11, OME16, RS14, WC11, XYW+14].

Grubbs [RS17].

GSK3 [LJL+11]. GTKDynamo [BTA+13].

GTP [SS13c].

guanidine [HRJ+14, HGP14, HRJ+15, JRSHP14].

guanidinium [CCCLCGRO14].

guanine [BZH14, LZH+11, PDM10].

guanine-cytosine [LZH+11].

guanines [WGL12].

guanylthiourea [MAPB10].

guest [OAN15b, YDGZ15].

GUI [WCJ+14, JCL+17, KLJ+17].

guide [BS15, GKV+13].

guided [OCL11, WBVE16, YVEI+17, Yon16, ZC14].

guiding [HS17].

gWEGA [YLGX14].
NMLD13, OPRI6, PMG^16, RMPAM15, SNDK16, STS^10, Tak11, TSJ^10, TFO^11, UT14, VIT^15, VV14, WKC10a, WLKC12, WHL^10, WWKS16, WCL^11, XFX^16, YKH15, YZ15b, YZZ^17, ZYLL12, AS15a, Ben17, BS10b, CK10, CKL^11, Chu10, DHE^12, GTK10, GS11, HZ11, HRL11, KTT16, LJW^11b, LWD13, Niz13, OKIS17, PTK11, Pie14, Pon10, STS^10, TS15a, UT15, WGL12, WvRSM14, XhD15, YZ15b, YZZ^17. H- [Pon10].

H-atom [BS10b]. H-bonding [WGL12]. H-C-C-H [YZZ^17, YZZ^17].


Heats [KSM16, ZWX^16]. headgroup [PS10]. headpiece [LKL10]. heat [MO15].


Heating [MO15]. Heats [KSM16, ZWX^16]. heavy [VKAM12, WS11]. heights [BS10b, KG15, ZW17].


Henry [QYL10, VKTRJ15]. HFO [HyL11]. hexagon [GHZ10].


Hessians [GVP^10]. heterobimetallic [DSdAR10]. heterocyclic [BSDP16, CWT^12, KYKR15, LXZ^10, RF15, SGHL13, WS12].

Heterodimer [YT12]. Heterogeneous [DSF17, AFPI13, CKKK16, YZZ^17]. Heuristic [Hel13, MS16, Tak10].


Hexhalogenated [VYJ15]. hexameric [RCM^13a, RML^15].

Hierarchical [JYC+16, BCG10, GBFD12, KKNN11, RMPAM15, SNS13].

High [MCLD10, MKB+13, RSLS13, BACSCJ+10, Cam15, CM13b, CSSB11, DH17, DLSD13, ESIB13, EWK+13, GWJPJ11, IPAA11, JBAM11, JC16, KSM16, LL10a, MJLV14a, MO17, OPB+12, PVL+13, PVJ10, RVCF13, REH13, SC15, WGL+11, WDLG12, ZWL13, dSAdSL13]. high-accuracy [RVCFF13].

High-level [MCLD10, EWK+13, KSM16, PVL+13].

high-order [REH13].

High-performance [RSLS13, CSSB11, EWK+13, LL10a].

high-precision [DH17].

high-pressure [WDLG12].

High-quality [MKB+13]. high-resolution [CM13b, JC16].


histogram [Fer17, HHWL17, SH11b, ZH12]. histone [GHK12, GH10a, GSD10, KC13a]. HIV [DLZ15, NNN16, OBW12, SYH12, TTB+10, UNT16, XLY12, ZaA10]. HIV-1 [DLZ15, NNN16, SYH12, TTB+10, UNT16, XLY12]. HIVgp41 [BAMR13].

HMH [LDJ+10]. HNCN [WLH11]. HNO [BLG10]. HOB [LCL+10]. hole [Cas13, CWHH11, EPH+13, GZZM16, GA12, LZL+15b, PAK17, PTB+15].

Holliday [Ish10, She12]. holographic [CDB10]. HolT [She12].


homology-model [KOY+12]. homology/ab [DJ13]. homonuclear [BWKW10a, BWKW10b]. homopeptides [FCD10]. HomoSAR [BPC13].

HONO [BLG10]. HOONO [BLG11]. hopping [JLH+14, KV14, LWZ+11, RDRc16, SRSLO15]. Horizontal [PC16].

hormone [HYYZ13, LLL+10, NS10, OME16]. hormone-dependent [NS10].


Hybrid [CGR16, KS15, ZDKM12, BTA+13, BG13, CCB15, CSK15, CC11, DR11, DJ13, FHT+15, GFG11, HOX17, JMS14, KN17, KKR+13, LBH+11, LT14, MIS+15, OK16, PW12, RSG14, SGPJS+17, Sea10, SXZ13a, SXZ13b, VI17, WN1M17, ZWLX11, ZWL13]. hybrid-meta [BG13]. hybridized [DC13].

Hybridizing [RDRc16, FZL+15]. hybrids [KM13]. hydratase [LT13].

Hydrated [ALH+10, BMFG16, CGPP11, GBL+11, GNGCA10, LPE+10,
hyperpolarizability [ISO+13, KBC12, Lu11, TKC+11, WXS+12, WZK+13].
hyperpolarizability [KSK11]. hypersurfaces [Ano10a, SN10]. hypervalent
[SLT14, SLT+15]. hypothesized [LLB+12]. hypoxanthine [FF11]. HZSM
[cCVG+14]. HZSM-5 [cCVG+14].

I50V [DLZ15]. I50V-induced [DLZ15]. IBIsCO [KVQC+11]. ice
[LPAS11, TD11]. icosahedral [FCW+14, GKSS14]. ID [LLHM16].
Identification [HRB+17, KYT+17, RLL+10, DL16, JSD+11, MPNS13,
RLDJ17, WSH10, YZWC11, ZYvIZ14]. identifier [hi12]. identifiers
[GPSM11, GPSM12]. identify [LLHM16, LHL+10]. Identifying
[AC12, HAGK10, XTY+14, LHO17, LLJ12, She12]. identity
[Höf14, KN17, YN15].

Illuminating [NSO+14]. illustrating [RML+15]. illustration [RP15].
Image [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g,
Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano12o,
Ano12p, Ano12q, Ano12r, Ano12s, Ano13a, Ano13b, Ano13c, Ano13d,
Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13k, Ano13m,
Ano13n, Ano13o, Ano13p, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u,
Ano13v, Ano13w, Ano13x, Ano13y, Ano13z, Ano13-27, Ano13-28,
Ano13-29, Ano13-30, Ano13-31, Ano13-32, Ano13-33, Ano13-34,
Ano13-41, Ano13-42, Ano13-43, Ano13-44, Ano13-45, Ano13-46,
Ano13-47, Ano13-48, Ano13-49]. Image
[Ano13-50, Ano13-51, Ano13-52, Ano13-53, Ano13-54, Ano13-55,
Ano13-56, Ano13-57, Ano13-58, Ano13-59, Ano13-60, Ano13-61,
Ano13-68, Ano13-69, Ano13-70, Ano13-71, Ano13-72, Ano13-73,
Ano13-74, Ano13-75, Ano13-76, Ano13-77, Ano13-78, Ano13-79,
Ano13-80, Ano13-81, Ano13-82, Ano13-83, Ano13-84, Ano13-85,
Ano13-86, Ano13-87, Ano13-88, Ano13-89, Ano13-90, Ano13-91,
Ano13-92, Ano13-93, Ano13-94, Ano13-95, Ano13-96, Ano13-97,
Ano13-98, Ano13-99]. Image


Implementations [LSD+10]. implemented [BVHI17, DLsA14, SR10, VBV13b]. Implementing [SCOJ13]. Implicit [CV12, CBG16, LP11b, LTP11, RB12]. Implicit [EM14, CAD16, Has14, CBG16, EKI5, FBEM11, KJDB12, KB11a, KB11b, LC17, ML14, SBW14, SLX+15, SCMA+17, TCC+13, WWKS11, YL13].

Kop16, Kop17a, Kop17b, KSR⁺¹⁶, Kow11, KVR10, LLH14, LPK16, LDJ⁺¹⁰, LJJ⁺¹¹, LPE⁺¹⁰, LX11, LJV⁺¹¹b, LLC12, LTP11, MK13b, MCLD10, MS12, NASH15, NMLD13, NDO⁺¹⁰, OHNK11, OYK⁺¹¹, ON14, OPR16, OT12, OZLSBH12, OOK11, PVL⁺¹³, DCOD13, RB13a, RFN15, SLT⁺¹⁵, SS13b, SLJB12, SLIZ⁺¹⁵, SLLL13, TLdG⁺¹², TG12b, US11, VV⁺¹⁵b, VPR10, WLC12, WXY14, WDHZ13, XZ11, Yu12b, Yu12a, ZZZ⁺¹², ZZ10, ZMM⁺¹², ZLT13, ZLZ⁺¹⁴, LL13a].

inito [JWST10].

Inner [KT12, HS16b].

Inner-[KT12]. inorganic [FNSF⁺¹¹, IGK16, OCW⁺¹⁵, SGH⁺¹⁶]. input [VV⁺¹⁵b]. insect [FCL⁺¹⁰].

insect-growth [FCL⁺¹⁰].

insertion [BB11a, LPK16, MG15, OLY17, WNM17, WHAS⁺¹⁰, WHAS⁺¹⁶]. Insight [CSM16, WC13, ZLHH14, CHKR10, DM15, LGWZ15, LZL⁺¹⁶, PM13, VIT⁺¹⁵, VBMA13, KKL⁺¹³]. Insights [EK15, FVP14, HRJ⁺¹⁴, HGHP14, HRJ⁺¹⁵, JRSHP14, RSB⁺¹³, ZWGO16, Alg17, GND⁺¹², HRMAL⁺¹³, HMS16, KP11, NDD10, OAN15b, PKK17, PSP15, RTS⁺¹³, SM16a, TN12, VV17, WM11, WDP⁺¹², YZ17, BTMS12, LJJ⁺¹¹]. inspection [KOY⁺¹²]. inspired [DSM⁺¹¹]. instantaneous [RO14a]. instanton [MRK11].

Insubria [GCC14]. Insulator [LLL⁺¹²]. Insulin [MV17]. INT [YJXZ13].

INT-DBD [YJXZ13]. integral [RFN15, SS13b, Sun15, VKAM12, WXY14]. integrals [CHC⁺¹³, PC16, SZTSM10].


Integration [FPV13, AYYO17, BB11b, BB11c, DH17, LP11a, MOS12, dRL11, Pol13, SJC11, SJ16, dRBO13]. integrative [Rez16]. integrator [JS17b]. intelligence [Aou16]. intelligent [CDS16].

Inter [CROB16, SS11, IHY15, SSB13]. Inter- [CROB16, SSB11, SSB13].

inter-residue [IHY15]. Interacting [CM16, EV14, HGCCGR⁺¹⁶, WL14].

Interaction [CK10, CCCLCGRO14, CCCLRO14, Den12, NNS15, SBW12, YZWC11, ALV⁺¹⁰, AG12, BLFZ13, BLF14, BCNH⁺¹¹, BHB⁺¹⁷, BRLS08, BRLS12, Cas13, CZH12, CYG⁺¹⁵, CTP13, EK17, EV14, FF11, FCCP17, GA14, GP11a, HBL12, HLM⁺¹², HSS⁺¹¹, JZMZ14, Kan15, KTNN10, LL10a, LMY⁺¹³, Li14a, Li14b, LHHW14, LZZ⁺¹⁵b, LPLB16, LCWW10, MSÅK12, OHPR17, OAN15b, PRJ⁺¹⁷, RZG⁺¹³, RS13, SM16a, SS13a, SBV10, SHF11, TYN15, WSH10, WYL⁺¹⁵, YK13, YWJ⁺¹⁶, YCK16, YHCS11, ZRC11, ZY14, KCB⁺¹²]. interaction-induced [BLFZ13].

Interactions [WCT⁺¹¹, ZCK⁺¹⁶, Abr11, ARRC15, AKK⁺¹⁶, AO10, CSS17, CIKT13, cCV⁺¹⁴, CKP10, CROB16, CB11a, CB11c, DHF⁺¹¹, DBG11, DLMH12, EP10, GWF11, GZM16, GZ14, HLvdV13, ICSC⁺¹², ICSC⁺¹³, IHY15, KSZH13, KCK⁺¹⁵, LZLC13, MLGB16, MKH⁺¹³, MR17, MJM⁺¹⁵, MVKS10, MG14, MFR⁺¹⁷, MPBJ11, OHNK11, PPJ14, PLV⁺¹¹, RTS⁺¹³, SSGS15, SDF12, SSB11, SSB13, TNSS17, TG12a, TY10, TSR⁺¹⁶, TNG⁺¹⁰, VV15, WS10, WGD⁺¹⁶, WM17, XTY⁺¹⁴, XLY12, YKO⁺¹¹, YZ15a, YW13, YZL⁺¹⁵, YDGZ15, ZZZ⁺¹², Zha11, dLC17]. Interactive [BRP⁺¹², BGR13].

interactiveness [CQFC10]. interatomic [DPAB16, FCCP17, YK0⁺¹¹, dLC17]. interconnections [GLF16].
iridium [CWT12, HDPM14, KB13]. Iridium-catalyzed [KB13].

Iron [HS14a, BG13, CTR13, GBGR16, HS16b, KPL13, KPL15, MC10, SBC+11, TS10b, VBMA13, EH13].


isocloso [LK16b]. isoconversional [DCS15]. isocyanide [TLY+12]. Isolated [FL15].

Irregular [Kan15, ALH+10]. k-Raman [Kan15, CWT12, HDPM14, KB13]. Irregular [Kan15, ALH+10]. k-Shrey [Kan15, CWT12, HDPM14, KB13].

Irregular [Kan15, ALH+10]. k-Raman [Kan15, CWT12, HDPM14, KB13]. Irregular [Kan15, ALH+10]. k-Shrey [Kan15, CWT12, HDPM14, KB13].

Irregular [Kan15, ALH+10]. k-Raman [Kan15, CWT12, HDPM14, KB13]. Irregular [Kan15, ALH+10]. k-Shrey [Kan15, CWT12, HDPM14, KB13].

Irregular [Kan15, ALH+10]. k-Raman [Kan15, CWT12, HDPM14, KB13]. Irregular [Kan15, ALH+10]. k-Shrey [Kan15, CWT12, HDPM14, KB13].

Irregular [Kan15, ALH+10]. k-Raman [Kan15, CWT12, HDPM14, KB13]. Irregular [Kan15, ALH+10]. k-Shrey [Kan15, CWT12, HDPM14, KB13].

Irregular [Kan15, ALH+10]. k-Raman [Kan15, CWT12, HDPM14, KB13]. Irregular [Kan15, ALH+10]. k-Shrey [Kan15, CWT12, HDPM14, KB13].
56

Material

[AW11, GPS10, HS12].

Materials

[BSL+16, CD11, DLT17, ECZW17, EMD17, Man13, NDD+10, SYZ+17, VBV13a, VBV13]. MATLAB [DKK14].

Matrices

[Car14, LHO17, Mat14, Yon16].

Matrix

[Car14, LHO17, Mat14, Yon16].

Matrix-based

[GGW11].

Matrix-free

[VBV13].

Maxima

[Luc14].

Maximum

[MLC13].

May

[SMGB11].

MBJLDA

[SRS14].

MC

[LL14a].

MC-DFT

[LL14a].

MCN

[LLL11].

MCQDPT

[LLSW14].

MD

[HCD+10, RSR+12, BM12, FB14b, GNASBF16, LL+11, MTvG12, OYK+11, RAR+11, SISK10, SMP17].

MDAnalysis

[MADWB11].

MDLab

[CCW10].

MDTRA

[PVZ13].

Mean

[ADG10].

Mean-force

[ADD10].

Meaning

[PSP15].

Means

[KSM16, TTB+10].

Measure

[WF16].

Measurement

[MPG11].

Mechanical

[ADG10].

Mechanical/effective

[DR11].

Mechanical/molecular

[SOY12].

Mechanical/dynamics

[ADG10].

Mechanical/generalized

[ADG10].

Mechanical/molecular

[ADG10].

Mechanics

[ADG10].

Mechanism

[GZL12, SLY+10, VKNT15, WCWW11, BNS14, BMFG16, \(B + 11\), CPV+12, CPLL11, FB14b, GY+10, GRLC12, HYYZ13, HDHL15a, HDHL15b, HDHL15c, JCG+10, JLS+10, JW16, KV14, KT12, KS13b, LZL+10, LZZH11, LLB+12, LWXC16, LHT15, LPMT17, NJJX+10, Oht16, PMT16, RLG11, SDK+15, LL13, SBLW12, VM10, WZ10, WCL+11, XLY12, YFC+10, YHG+11, ZSWL12].

Mechanisms

[ADG10].

Mechanistic

[LZL+16, TSJ+10, YZ17, ABB+12, ABB+13, GND+12, NG14, WHLZ11, YZG014b].

Mechanochemical

[QB16].

Mediated

[MRR11, RVP+11, XYW+14].

Medium

[FE14, IPA11, RK15, WW14].

Medium-size

[FE14].

Medium-sized

[RK15, WW14].

Melanin

[LLL+10].

Melanin-concentrating

[LLL+10].

Mellitus

[PC11].

Melting

[FCW+14].

Membered
Methodological [VKNT16]. methodologies [Rob13]. methodology [Aki16, FF11, GAI13, GMASBF16, OHPR17, RJWW12, HCD+10]. methods [Ano12u, Ano15-59, ASMS10, BG13, CSGOA17, CXS10, CNK97, DBM+15, EWK+13, ESM+12, EV14, Fer13b, Fer13a, FB10, FSSW17, GAI14, GFPSD17, GD10, GSS13, GMO16, HCB11, HSB+11, Höf14, HWLW11, JJJ+13, KB13, KHWB17, LaEdOLdV17, LZLC13, LLSW14, MS13, MY17b, MR17, MVKS10, MOS12, NASH15, NC13, NC14, NTNY15, OSHG17, DCOD13, PN13, PVAM16, RZG+13, RRH12, SRF+17, ŠSB+16, SACdG14, STM+15, SGWA17, TG12b, Ts15b, Ts17, WBT10, WX12, YLCX10, YAS13, YJ17, ZGS+10].
modulators [SRA17]. module [PHH+12, VBV13b]. MOFs [LPK16].
MOLCAS [ADF+10, VBV13b, AAC+16]. Moldyn [HPSK12]. Molecular
[BDTP11, CMD13, DGH+11, DSD+11, DHF+11, Fom13, Ibr11, JA10,
KUDG12, KB14a, LWZK13, LBPD12, MFEM16, PL14, Pla11, RKGN10,
RO14a, RRK14, SB17, SV11, VSD10, WC11, WWKS11, XFG+16, XLY12,
Yan16, YJXZ13, ZWS+10, AALCM11, AG11, AST+16, AFP13, AS15a,
ASL+11, AS10, APK14, AGB13, AS15b, AGR11b, AJR16, AB16a, ALH+10,
BMR11, BAMR13, BEM14, BS11, BF15, BBOB16, BJSI12, BV14, BW15,
Bjp15, BMBJ11, BE16, BC13, BEL+11, CBP14, CM13a, CDBM11, CD13,
Car14, CF13, CAF+13, CEB15, CIKT13, CGPP11, CS14, CXW14,
CBTZ16, CH16, CC1H14, CV14, CCW+10, CHKR10, CB11b, CB11c,
CM16, DSD+11, DJX+11b, DJX+11a, DLZ15, DDM+15, DL16, EP10, EK15,
EJ13, EPH+13, ENKK+17, EPD+11, FBM11, FSC+14, GBL+11, GDV17,
Gar12, GJM14+14, GSHM10, GR11]. molecular
[GMZ12, GM14, GM14, GM14, GP+14, GP+14, GP11b, GR10b, GP12, EP+15, HB14, HS12,
HCD+10, HDM+15, HPSK12, HH16b, HHLW11, HJ10, HXM+16, HHWL17,
HR16, HC14, IUK+10, II10, JIS13, JBSQG11, JAH+17, JSXH16,
JWST10, JGS17, K10, K10, K10, K10, K10, K10, K10, K10, K10,
K10, MJC14, MCRL17, Mat10, Mat14, MSV+12, MFT+15, MADWB11, MPNS13, MKM+17, MBA14,
MR11, MCC12, MFR+17, MO17, MS12, NPTS16]. molecular
[NSO+14, NLP+16, NST14, NPG17, NF17, NFG+13, NF17, NNK+16,
NHK+13, NS17, NTN15, Oht16, OHNK11, ON14, OGL10, OHP17,
OCL11, OLY17, OT12, OME16, OVPK15, OOT15, OCW+15, OZS+13,
OOK11, PMC+17, PSS14, PAK15, PAK17, PH17, PM13, PGW+17, PV13,
PB13, PS10, PV16, PLP+16, Pro16, PH15, PVJ14, RMP15, RLLH12,
RSF+16, RNP13, RNVP13, RS12, Ras17, RHJ11, RO14b, RR14, RL14,
RSH15, REH13, SHMO11, SLE+15, Sax12, SMV10, SK15b, SA13,
SZS10, Sch12, SF+11, SHF11, SFRM+17, SOM+13, SJ17, SY+12,
SK3, SWB+12, SLLE13, SJ16, SDS13, SKY+11, SBvG14, SA15,
TNYN16, TKNN10, TZ12, US11, VYM15, VBM11, Vb10, Vb12, VM11,
WKLC12, WBN+13, WAM17, WLW+10, WH11, WCY+11, WLC12, WOH16,
WX17, WES13, WBF17, WCDM11, WO15]. molecular
[WCW15, WL14, WGI4, XDL+10, XFG+15, YPD13, YNH+17, YL14,
YLCX10, Ynp11, YPK12, Yes12, Yes15, Yon16, ZST14, ZW13, ZZY+16,
ZX11, ZDKM12, ZSS+13, ZLY+16, ZP13, ZWX16, ZLL+13, ZA15,
ZBMZH15, dCLFL13, IPAA11, KSD+12, MJL14b, ZBP11, ZK+10].
Molecular networks [MCC12]. Molecule
[KR12, vRWGS17, DHOG13, DGL+13, ETLS17, FAA15, GAI14, GCWS15, GBVA11, HLvdV13, HHWL17, ISO+13, IIHY15, KB11b, LIRL+16, MCUJ15, PCLL11, RLL+10, SG10b, VGV+11, WF16, XYW+14, XMSZ16], molecule-mediated [XYW+14]. Molecule-specific [KR12]. Molecule-transcription [XMSZ16]. molecules [AIGP15, ARAG17, AGR11a, BLBG+13, BS10a, BTMS12, Ben17, BS16b, BL12, CHG+16, CQFC10, CYG+15, COOH14, CXS10, CZNA11, FE14, GWF11, GP12, GPGSM11, GPGSM12, HRB+17, HSB+11, Hug12, Ihl12, Kan15, KLJ+17, KYG+15, LPS12, LHSH12, LvG13b, LH14b, LJL+11, LG14, MA16, MS13, Mat10, MSS+13, MBE16, MPBJ11, NIIT15, OGL10, OT12, PZBA13, Pyy13, RSG14, RK15, SFCCK+14, SFCCK+15, Sch13, SG10b, SY16b, SM17, TSN+16, UNT16, VVV+15a, VHA+10, VDVR14, WC13, WSWZ15, WWD14, WX12, Yot10, YKH15, YHW17, ZPP+16, Zha12b, ZLX+13, ZBB16, ZCGM11].


Mulliken [BVC13]. Multi

N
[Ano15-59, BLF14, BCNH†11, KBC12, KCL†14, LPLB16, NDG14, PVL†13, BCNH†11, BWKW10b, BMB13, BSDP16, CWT†12, CCM15, DCHL12, DFW12, GMASBF16, GZL†12, HLH†12, KV14, KCL†14, LZZH15, MLGB16, MS15, OZLSBH12, PVL†13, RHNN10, RWR†13, SGHL13, TSJ†10, VM11, WS10, WGL†11, WCL†11, WYGW12, WS12, Yu12b, ZP13, HPSK12].

PW12, PPM15, PHH+12, PVZ13, PG14, RLLHL12, RNSF+16, Ras17.

News [Rez16, RR14, Ra1A2, RSR+12, RCM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sie15, SJ17, SWB+12, SDMS13, TNYN16, TSC+13, TTR+12, TTL+12, UU12, VMRS+17, VVV+15b, VARI12, VBV13h, WdVNI2, Wdy13, WPM+15, WF16, Wei12b, WHK+12, WHJJ13, WG14, WCI+14, XM+15, XYX17, YWJ+16, YZZ16, Yes12, Yes15, YHH+13, ZDKM12, ZLL+13, dVAG16, KKR+13]. Next [ADF+10, HGY15].

next-generation [HGY15]. NF [ABB+13, ABB+12], NGuaS [WGN+16, WLG+16, WRG+17]. Nguyen [Ano15-59], NH [CG12, KSK11, LBTV12, CCJ+11, Kopp15a, LYC+13, LBT11, ONTTL16, UT14, Yu12a].

NH … [MVKS10]. NHH [LZH+11]. NHOC [LHHW14], Ni [TLdG+12, Tsi17, WWKS16, MMB+17, SSX+14, TLA10, ZRCC12]. Ni-NO [Tsi17]. nickel [ED15, FCW+14], nicotine [PMC+17], nitrate [OS10].

nitric [BS16a], nitride [GLF16, LT14], nitrides [TS11], nitritolotri [CM16], nitritoloti- [CM16], nitritolatriacet [CM16]. nitro [YPC+10, ZW11].
nitro-substituted [YPC+10], nitroalcohol [QLYL16].

nitroaniline [ZTH+15]. nitroaromatic [PSC11, TD10].
nitrobenzenes [ZGS+10].
nitrocompounds [SIG+15, STH+16]. nitrobenzofuran [DPB+12].
nitroethane [YZL+15].

Nitrogen [LLC17, BEMP14, KY14, ZZWX11, ZYL+12]. nitrogen-atom [KV14].

Nitrogen-doped [LLC17]. nitrogen-rich [ZZWX11, ZYL+12].
nitrogen-substituted [BEMP14]. nitroiminoazotetrazolate [ZYL+12].
nitromethane [MCU15]. nitrosamine [dALdS+15]. nitroso [TDP+12].
nitrosothiol [TKXT13]. NMR [Ben17, CHP11, EOA+11, HJ13, HBI+17, HM13, KASH14, LKK11, OPR16, PTK11, PGdO+16, PC14, P1e14, RK15, SF+16, SKMS13, WL14, YS13].

NNO [WGL+11].

[MCU15, Tsi17, ZZ10, WYGW12, BS16a, GY12, OSH17].
noble [ARLP13, JKS+16, PGS+15, PMG+16]. NOCV [CSM16].
nodes [KK17a].
nodes [KPF+15]. NOEs [LK11]. Non

[KB11c, LCH10, CSKH15, GMZ12, MR17, NHN16, PHC13, RS13, YWJ+16]. Non-Boltzmann [KB11c]. Non-Born [KCH10]. non-covalent [MR17, RS13]. non-equilibrium [NHN16].
non-heme [PHC13].
non-hybrid [CSKH15]. non-natural [GMZ12].
non-uniform [YWJ+16].
nonadditive [RTS+13]. Nonadiabatic [HZ11, JBSQ11, SRSLO15].

Nonclassical [GZH10, DM15].
noncovalent [RRH12, SM16a, SBW12, TS+16, VT14, WGD+16, YW13].

noncyclic [SM16a].
nonempirical [WT17]. nonequilibrium [ASL+11, KHW17].

Nonfitting [RZG+13].
nongeometric [KB11a].
nonheme [BG13].

Nonideality [GC11].
nionic [WWKS11].
noniterative [MS12].
nonlinear [ARLP13, KOP+14, LLD17, MLQ+12, MIS+15, RLA+11, TFQ+10, Tia12, YCGA10].
nonlinear-optical [KOP+14].
nonlocal [LPAS11].
nonlocality [FVB10].
nonorthogonal [ZM11].
nonparametric

nylon [BHNS14]. nylon-oligomer [BHNS14].


[SH11a, AMGB10, Ant13, CX10, NMLD13, RVP+11]. **pathway**
[BHB12, HOM+16, LKL10, SJD14, TDP+12, XLYZ10]. **pathways**
[CM13a, EFB16, GS11, HNTS15, KGR+16, MTM14, QSW+10, QB16, RCM+13a, RML+15, SJID11, Ts17, WSH10, Yon16, BHB12]. **pattern**
[CXS10, WGL12]. **patterns** [FZL+15, RS14]. **Pauli** [Ano15-60, Ano16-56].

**Pauli** [JH+13]. **PAW** [MDTD13]. Pb
[MCK17b, PMG+16, vSGP10, FBY+17, OBW12, vSGP10]. **PB-AM**
[FBY+17]. **PBE** [DOM+11, PTK11, LK16a, SGPJS+17, TG12a].

**PBE-QIDH** [SGPJS+17]. **PBE/3z** [PTK11]. **PBE0**
[DOM+11, LK16a, SGPJS+17]. **PBE0-DH** [SGPJS+17]. **PBESOL**
[DOM+11]. **PBSA** [CS17, RDDS10, STM+15]. **PBSS**
[DVVP14]. **PCASSO** [LFB14]. **PCCP** [VT14]. **pCCSD**
[Sch12]. **PD**
[HLS+13, Hil13, KD10, Niz13, YDR13]. **PD-PK-T** [HLS+13]. **PDB2PQR**
[UHH+11]. **PDBbind** [PLAG11]. **PDECO** [CJL+13]. **PDIELEC**
[KB16]. **peaks** [LZS+17]. **PEG** [EEO+16]. **PEG-PLA** [EEO+16]. **penalty** [GZH10].
[RRF11, ZKH+10, OOk11, ZZY+16, GRS15, RN12], **ab** [DJ13].

**ammonium** [AvKSP16]. **aromatic** [MJM+15]. **AT-rich** [YWC11].
**aug-CC-pVTZ** [Gil11]. **back-bonding** [PPK17]. **basis** [PD11]. **Brownian**
[DMN15]. **CASPT2** [LWGZ15]. **cholesterol** [RBOH11]. **configuration**
[FF11]. **D** [Chu10, KTT16, UT15]. **D5Cost** [REL+14]. **DF**
[Chu10]. **DFT**
[BRLS12, BRLS08]. **dissimilarity** [YDL+10]. **DSiCl** [LX11]. **dynamics**
[DDM+15, EPH+13, GPdC+16]. **E-I** [GM17]. **effective** [DR11]. **Fe**
[DAadGR15]. **FEPL** [HYUS11]. **GBSA** [GR10a]. **generalized** [HWLW11].

**GIAO-CCSD** [ORF16]. **GULP** [SN16a]. **hydride** [PM13]. **hydrophilic**
[PAX15]. **II** [KPL15]. **KCl** [HB15]. **Kohn** [VV14]. **lithium** [EK15].
**local** [SB15]. **MC** [HYUS11]. **MC-XQDPT2** [KKL+13]. **MgO** [BS16b].
**MM**
[BM12, AALCM11, BTA+13, CZY11, CJZS10, DSK17, DSX+11, FLM11, FDB12, FB14b, GWZ15, GCW14, HH15, HBR17, JH+13, JSTW10, KTN10, KWL+16, KWG15, LFM12, LT13, LHT15, LJJ+11, MCR17, MTvG12, MJG+15, NO16, PMC+17, PDMT10, PL14, RR14, RN17, RR12, SN16a, SGDT10, SJID14, SCM+15, STM+15, SSAS10, TSC+13, VKN15, VKNT16, VCM15, VKTRJ15, WDP+12]. **MM-MD** [RSR+12, OYK+11].

**MM-QMC** [UTM11]. **molecular**
[BEL+11, Fer13b, Fer13a, RdA12, YKO+11]. **multiple** [JS17b]. **NaCl**
[HB15]. **nucleophilicity** [TMJ15]. **OD** [Chu10]. **oligomerization** [KAR12].
**OpenMP** [KS15, KN17]. **or** [KB10, Pog10]. **PB** [VM11]. **PBSA**
[BD11]. **PC** [VL17b]. **PCM** [LFN+10]. **PC-MST** [GMMH+16]. **phenol**
[IYY11]. **phosphorus** [GWX+12]. **Poisson** [HWLW11]. **QM+**
[PLP+16]. **QSPR** [CLX+10, GCC14]. **reaction** [KSK1]. **repulsive** [SN16]. **SAC-CI**
[EFS16, IN13]. **superoxo** [ZRCC12]. **TD** [TS15b]. **TD-DFT** [LXZ+10].

**TDDFT** [MS11]. **thymine** [HV12]. **time-dependent** [JYS+12]. **TIP3P**
[SA10]. **uracil** [HV12]. **vacancies** [HRB+17]. **Vis** [GGM+12]. **water**
[JA10, SV11]. **Zn** [GEP+14]. **penetration** [NL+16]. **Pentaatomic**
[XH15]. **pentacene** [CWHH11, ZYG+15]. **pentacoordinated** [TS10b].
pentagon [FL15, GZH10]. pentaprismane [PCLL11]. pentathienoacene [ZYG+15]. peptide
[FP17a, HPL13, HLH+12, ICS+12, ICS+13, JBAM11, JWST10, LTT16,
LW11, LlvG10, LJW+11b, LvG13a, LMA15, MDT10, MV17, OZ14, QZM11,
SV15, SEM12, TYZ+16, XHLH16, YZ15a, dCLFGL13]. peptide-backbone
[HLH+12]. peptide-design [XHLH16]. peptides [BLKP12, BPC13,
CCOH14, CZNA11, GF11, HLH+12, HHWL17, IO13b, JCYX10, KB10,
Lw11, LLvG10, LJW+11b, LvG13a, MZZ11, OLY17, XHLH16, XWSW13, ZKH+10]. peptoid
[MMZW14]. perception [AJR16, HYYZ13]. Performance
[Abr11, BZB+13, CSKH16, CKKK16, DOM+11, HSB+11, JCP14, LK16a,
RKb+14, SGWA17, ABM+15, BLBG+13, CXS10, CSSB11, CJS10, ESB13,
EWK+13, GAI14, GRAR0+14, GSS13, HMLW11, KZZ+16, LL10a, LRBB12,
LC+10, MC12, MG11, OPB+12, RRH12, RSL13, SRF+17, SPR+13, SJ16,
TF15, YPC+10, ZSL17, ZWL13, SBW12]. Pericyclic
[HPT16a, KG15]. Periodic [Sce07, Sch10, AAC+16, CEBO15, FCD10, Gar12, HSH15, HBI+17,
ITIN15, KB14a, LBGS16, Man13, MGS+16, NO16, NTNY15, RJPB12,
SN16a, SE15, TLdG+12, Tak14, VBV13a, VBV13, VECT12, VI17]. Perlin
[HLBLCCG15]. permeation [DNM15]. permutation [IO13b]. pernitrides
[WD10]. peroxo [RHPWS13, RHT+15, ZRCC12]. peroxo/superoxo
[ZRCC12]. peroxyinitrous [BLG11]. persistence [WX15]. Persistent
[XFTW15]. perspective [ABDGN12, DI15, Hsu14, JCGVPHT17, JMX+16, LGOM+15,
Niz13, PM15, XLY12]. perspectives [DR14, Wei12a]. perturbation
[CMM15, CF14, DCHL12, FRSA14, FSSW17, FE14, GRS15, GCCM15, HIL13,
HRJ+14, HRJ+15, HYUS11, JRSH14, KKNN11, KN17, KM13, LCL+10,
LlvG10, LGL11, LlvG13b, Lg13a, MCCI11, RLDJ17, RAR+11, RHPWS13,
SSSM15, TAG16, VDL+13, WHAS+10, YKH15, ZSL14, WHAS+16]. perturbation-selection
[FE14]. perturbations
[GMSdG15, OS16, Tak10, WWCL15]. Perturbative [SSWX14]. perylene
[BSL+16, SLP+12]. perylenediimides [QCR12]. pesticide
[BHB+17]. peta [KNHN16]. peta-scale [KNHN16]. petascale
[SCOJ13, ZWL13]. PH [LZL+15b, dSDdAR10, LZL+15b, AB16a, CS14,
CAD16, HS14b, MBA14, PZA15, PS13, SY16a, SOvG12, VR12].
pH-dependent [SY16a]. pH-responsive [MBA14]. Phase
[MP17]. Phage-like [MP17]. PHAISTOS [BFH+13]. pharmacokinetics
[VBD+11]. Pharmacophore [HRK+10, HKRS11, HS11, TD10, AKMT11].
Phase [ZWMW10, ABB+12, BE12, DLS13, DLW12, EMD17, GYX+10,
Hsu14, KD10, LJJ11a, LPLB16, MF+12, NIT15, PSC11, RWR+13,
RSLML12, RJ17, SJZ+15, VKAM12, VED10, YHG+11, YGS12, ZSV+14,
ZWW10, ZYR+15, ZLHH14, dSDS12a, dSDS12b, ABB+13]. phase-change
[EMD17]. phases [EB12, LPAS11]. Phen [FD16]. phenol
[AAMD+11, AK10, PPH+14, WHX+10, YKH+10, AK10].
phenol-imidazole-base [YKH+10]. phenol-triethylgermanium
[WHX+10]. phenolates [SKGB13]. phenols [SK12]. phenomena
phenyl [GZL+12, ZWY+10a]. phenylacetylene [ZZL+12].
phenylacetylene-containing [ZZL+12]. phenylalanine [GWF11, PVS12].
phosphaalkene [TR12]. phosphano [KYKR15].
phosphate [MRO17, XZ11, YZGS14a]. phosphatidylcholine [PVM10].
phosphetane [SHL+13]. phosphine [MG14, YK13]. phosphorous [KLN12].
phosphorus [RB12, YDX16]. phosphorus-containing [YDX16].
phosphorylation [RIJ+11]. photolysis [HNN+17]. photophysical [CWT+12].
phthalocyanine [SKY+11]. phycocyanin [RCM+13a].
phylogenetic [CCYL11]. phytochrome [FD13]. piano [FPB12, FB14b, ZCK+16].
piano-stool [FPB12, FB14b, ZCK+16]. pictures [MA16]. PICVib
plage [SSSM15]. Pimpehales [TTL+12]. pinane [BLS10]. pincer
[ED15, JJB16]. pincers [KJD16]. pinene [BLS10]. Pipek [HJJ13]. PK
[HLS+13, GK15a, SK15a, SK12, SK17, YDX16, Zha12b, Zha12a]. PLA
[EOO+16]. Placevent [SYH12]. planar
[BSPP+13, EV14, XhDi15, ZYW+16, ZLY+16]. Plane
[SH14, BTB+11, EH13, Gav12, LL13b, MDTD13, MDTD16, TCB16].
Planar-wave [SH14, BTB+11, MDTD13, MDTD16]. plasmapin [SOD+11].
plasmigen [BM12]. plasmon [Ano15-58, BH14]. plastocyanin [HBR17].
PLATiform [TNYN16, BTMS12, HPT+16b, PZCL16, VMRSH+17].
platforms [SCOJ13]. platonic [KSM16]. PLATYpus [TNYN16]. plausible
[KV14]. pleated [WCAH10]. Plesset
[FSSW17, HI13, KKNN11, KN17, MCC11, YKH15]. PlmII [VLB+10].
PlmII-inhibitors [VLB+10]. plug [BTA+13, KLOS10]. plug-in
[BTA+13, KLOS10]. Plugin [BHB12]. plumbacyclopentadienylidenes
[KASH14]. PM3 [SA10]. PM3-CARB1 [SA10]. PM3-CARB1/TIP3P
[SA10]. PM6 [SBW12]. PM6-DH2 [SBW12]. PMF [ZLX+13]. PMMA
post-translationally [MRO17]. postprocessing [HPT⁺16b].
posttranslational [Ano12u]. potassium [SG10b]. potent [NS10, XDL⁺10].
Potential [Vor12, AMGB10, BTA⁺13, BLF14, BPM15, BBI⁺11, CM13a, CG15, Car14, CKP10, CKKK16, DR11, DLT17, DS12b, DLSA14, EFS16, EPH⁺13, FMNC11, GKV⁺13, GLM⁺17, GKSS14, GA12, GFG11, HDL⁺17, HBKL10, HYD10, KS13a, KS15, KTT16, KPL13, KPL15, KERY⁺16, KS12, Kop15a, Kop16, Kop17a, Kop17b, KGM12, KYG⁺15, KCL⁺14, uLhY11, Lar11, LYG⁺13, LX11, LSH⁺11, LCM16, MK13b, Mat14, MPNS13, MB14, MLCD11, NNS15, NW17, OKIS17, PRRT⁺10, RLD12, Ri10, SBR13, SN15, SRF⁺17, SC15, SSB⁺16, SRS14, SLG15, SJ16, TBSM12, VMRSH⁺17, VOT14, VLI17a, VOT16, Vy15, Vy16, WKC⁺10b, WLO⁺17, XFX⁺16, Yu12b, ZDM13, ZLT13, ZWF15, ZGS⁺10]. potential-derived [TBSM12].
Prediction [Ano12u, CP15, CQFC10, HZSS17, KPL15, MA6⁺16, yOaCG10, PRP15, SRA17, WD12, YW17, ZYL⁺12, AGM⁺13, BLDK⁺13, Ben17, BDdIS13, BA11, CZAF17, DWL11, DDP16, EOÄ⁺11, FZY⁺12, GK10, GFPSD17, HLS⁺13, HYM16, HL14, JSW10, KLI4, KT10, KTO11, LXL⁺11, LMY⁺14, LZZ15a, LZZ14, LLI11, LWL⁺10, LSH⁺11, MDT10, Mau14, MG11, MSÅK12, PML⁺12, PN13, PPJ14, PLV⁺11, RCR⁺16, RKB⁺14, SM11, SYH12, TYZ⁺16, VKC10, WLF11, WH11, WXS⁺12, WX1⁺12, XFTW15, YVEI⁺17, YLCX10, YHH⁺13, YDX16, YDZG15, ZsA10, wZbZ11, ZYvI14, ZL10, ZHX11, VVBL17].
principle [CCJC10, DBM+15, LLB+12, MCF10, Tak11, YPvD13].

**Principles** [HFSO12, BE12, BE14, BPE16, EMD17, EB12, EBK13, GD10, HYL+11, JCG+11, LLLM11, LCWW10, NNS15, RZG+13, TZ11, WYL+15, WD10, YR13, wZbZ11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC+14].

**principles-based** [Zha12b, Zha12a].

**prismane** [DM15, VIT+15].

**Pro** [RB12].

**Pro-Tide** [RB12].

**probe** [RN17].

**Probing** [HH15, KG11, LPK16, TG12b, ZYR+15].

**ProBiS** [KDT+12].

**problem** [HFSO12, BE12, BE14, BPE16, EMD17, EB12, EBK13, GD10, HYL+11, JCG+11, LLLM11, LCWW10, NNS15, RZG+13, TZ11, WYL+15, WD10, YR13, wZbZ11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC+14].

**problems** [PNW+16].

**procedure** [AC11b, KSM16, PW12].

**procedures** [AD10, BKS+11, BY11, CJZS10, HKR+14, MG14, MS12, SA13, dSAdSL13].

**procedures** [AC11b, KSM16, PW12].

**process** [AB16a, AB16b, BDTP11, Fom11].

**processes** [AC11b, KSM16, PW12].

**processing** [AK10, BS16a, KTT16, XML+15].

**processor** [HKR12].

**processors** [AC11b, KSM16, PW12].

**produced** [LS11a, SIG+15].

**Producing** [RN17].

**produced** [LS11a, SIG+15].

**produced** [LS11a, SIG+15].

**production** [LLC+10, PGL+15, PLAG11, vW11].

**proguanil** [APA+14].

**Projected** [EFS16].

**projection** [MDS13, RHRCH16].

**projector** [BVH17].

**prolapse** [TH13].

**proline** [AS11, HJLv16, OOK11].

**proline-catalyzed** [HJLv16].

**proline-recognition** [OOK11].

**promelas** [TTL+12].

**promising** [KSSH13, ZSL17].

**promolecular** [REV+17].

**promoted** [LPLB16].

**Proof** [FVB10].

**propagator** [WWD14, YD17].

**propene** [HSL+11, QSW+10, dSDdAR10].

**Properties** [SFCK+14, TY10, ARAG17, ASS10, ARLP13, ALH+10, BCSCJ+13, BE12, BPE16, BLFZ13, BS10a, BACSCJ+10, BC13, CBH14, CWT+12, CWHH11, CBTZ16, CH10, CCYL11, CXS10, CLC11, DDP16, DOM+11, DBM+15, DPNM11, DJX+11b, DJX+11a, DP15, DLW12, DQ16, FB10, GBL+11, GTT10, GKS10, GWJ+12, GBGR16, EPH+15, HZY+10, HRB+17, HLH+12, HSS17, HLWD15, JBSQG11, JJJ+13, KKPT11, KDB13, KZK+12, uLHy11, LHL+10, LLS12, LLLM11, LZJ+11, LLD17, LBT11, LBT12, LXZ+10, LWWG12, MCI10, MCF10, MJLV14b, Mat10, Mat14, MIS+15, MGS+16, MCK17a, NSO+14, NC14, PHC13, PGY15, PPK17, PGW+17, Pog10, PH10b, PBE16, PS10, RR14, RRF11, RI10, SDF+17, SB11, SLIB12, SWMW10, SIG+15, SGH+16, TN12, TFQ+10, TFQ+11, TS11, TS15b, VPR10, VECT12, WLC12, YW12, YCGA10, wZbZ11, ZYG+15, ZWMW10, ZLX+13].
properties [ZBP11, ZYL+12, SFCCK+15]. property
[CD13, GPS10, GBS+17, GWX+12, PH15, VAA14, WH11]. propionate
protease [DLZ15, NHN16, OBW12, SYH12]. protection [SBW12].
protective [JAH+17]. Protegrin [RI10]. Protegrin-1 [RI10]. Protein
[CIKT13, CDS16, DPOS16, GPS10, HNTS15, HS16b, LZGS11, MFEM16,
MFR10, PGL+15, Ran12, RP15, Rao11, SHMO11, SKKS13, AIGP15,
AKK+16, AM10, AG12, BSZ+12, BFH+13, BPB11, BPC13, BCG10, Bow16,
BddS13, BA11, CZAF17, CFC15, CHR+12b, CHR+12a, CM13b, CCYL11,
CKP10, CH14, CC12b, CBG16, CHP11, DLW11, DJ13, DVVP14, DLMH12,
FZY+12, FHW+11, FCE15, FLMI1, FSC+14, GS14, GDV17, GMSdG15,
GRP+12, GZ14, GRL+11, GRL+12, HAGK10, HNHR13, HTS15, HTS17,
Has14, HZY+10, HK12, HYMZ16, HJ10, HHBY10, HM13, HZ13, ILKR11,
IIHY15, JZ12, JZZM14, JL+17, KYT+17, Kan15, KNE11a, KOY+12, KL14,
KERY+16, KJ10, KTO11, KTO13, KDT+12, KLS10, KMLS10, LS11a, LFB14,
LHL+10, LH11, LCPS13, LC16, LC17, LZ11, LLC+10, LL10b, LFM12, LPS+13,
LZZ14, LLCL11, LHLG11, LBS10, LDH+14, MS17, MMM+16, MJCI4, MA14].
protein [MA17, MFEM15, MS16, MP11, MB13, MOS12, MNNK10a, NST14,
NS11, NFG+13, NG10, OHNK11, OCL11, OL13, OXBW16, OCLM14, OK16,
OME16, OOT15, PGCT+12, PGW+17, PLV+11, RZG+13, RCR+16, SBB10,
SYDS11, SK17, SM+13, SY16a, Sti15, TYZ+16, TNYN16, TNSS17, TRA+16,
TJB12, UNT16, UCFT16, WdVN12, WNP+16, WZ17, WES13, WHAS+10,
WHAS+16, XML+15, YZ15a, YZ16, YDL+10, Yon16, YS10, YL13, ZL11,
ZC14, ZYvZ14, ZLW10, ZLX+13, ZSB+16, dRBO13, LGL11, SL10, SHL+11].
ILKR11]. protein-ligand
[AG12, CHR+12b, CHR+12a, LLC+10, OOT15, WdVN12, dRBO13].
protein-like [KOY+12]. protein-lipid [PGCT+12]. Protein-protein
[CIKT13, JZZM14]. proteins [ABD11, CTR13, CGBK13, FZL+15, FP17b,
FBEM11, HS16a, Ham11, HTS15, HTS17, HRC13, HS14b, HRH+17, JC16,
JX10, LHO17, MBT14, NOS+14, NR11, OCLM14, yOaCG10, PGCT+12,
PRP15, PHC13, PNI13, PZBA13, PS13, SK15a, SA11, VMRSH+17, Vor12,
XSZL11, YZWC11, YMP14, DZA11, GREAI11]. proteochemometric
[NSO+14]. proteoglycans [NPG17]. proteolysis [VKNT15]. Proteus
[SGM+13]. protic [RK16a, RK16b]. protocol
[KPL13, RCR+16, SDL14, WdVN12, dCLFGL13]. protocols
[CLA16, EOA+11, GR11, ZKH+10]. Proton
[AK10, IYK11, RJWW12, RK16b, CG15, LPAS11, LBC+12, LZL+10,
LGZ15, MPSG11, RSB+13, SRF+17, SV11, TM16, VMTL10, Vor12, WG14,
YZGS14a, YKH+10, YYT12, dALdS+15, RK16a]. Proton-coupled [IYK11].
proton-ordered [LPAS11]. protonatable [Kan15]. protonated
[RSB+13, US11, ZLHH14, dALdS+15]. protonation
Q [WPM+15, BS10c, GKV+13], Q-CHEM [GKV+13], Q-Dock [BS10c], Q2MM [LN15], Q5 [REL+14], Q5/D5Cost [REL+14], QB3 [KG15], QC [BTA+13], QC/MM [BTA+13], QCT [BLG10], QIDH [MGJ17], QikProp [LP11a], QM [BM12, Lun12, SRS+12, RSR+12, Lun12, AALCM11, BH13, BZH14, CJZS10, DSK17, FLM11, FB12, FB14b, GRS15, GWZ15, GSW14, HH15, HYUS11, HBR17, JHH+13, JST10, KTN10, KW1+16, KWG15, LZJ+12, LDM12, LT13, LT15, LNL+15, MCRL17, MTvG12, MJG+15, NO16, OYK+11, PMC+12, PP10, PDMT10, PL14, PLP+16, RR14, RR12, SN16a, SGD10, SJ14, SC+15, ST1+15, SSAS10, TSC+13, UTM11, VKN15, VKN16, VCM15, VKN15, WDP+12, GRS15, RFN15, ZZY+16], QM-only [LT13], QM/MM [BM12, RSR+12, AALCM11, CJZS10, DSK17, FLM11, FB12, FB14b, GWZ15, GSW14, HH15, HBR17, JHH+13, JST10, KTN10, KW1+16, KWG15, LDM12, LT13, LT15, LNL+15, MCRL17, MTvG12, MJG+15, NO16, OYK+11, PMC+12, PDMT10, PL14, RR14, RR12, SN16a, SGD10, SJ14, SC+15, ST1+15, SSAS10, TSC+13, UTM11, VKN15, VKN16, VCM15, WDP+12, QM/MM-MD [RSR+12, OYK+11], QM/MM-QMC [UTM11], QM/QM* [PLP+16], QMC [UTM11], QMX [KKR+13], QSAR [GKR13, Ray13, AKMT11, BF15, CLX+10, FCL+10, GMHH+16, GCC14, LS1+10, LZL+15a, PKIC11, PPUBGD10, RKG11, TTB+10, SSL+12, WMW+10], QSAR/QSPR [CLX+10, GCC14], QSARINS [GCP+13, GCC14], QSARINS-chem [GCC14], QSPR
Recasting [RHRCH16]. receptor [CV12, ESB13, FTW12, FRLN10, HYZY13, ILKR11, LZ11, LLI+10, OME16, PPJ14, SSP+13, VKC10, WC11, YZZ16]. receptor-ligand [FTW12].

receptors [DR14, SRA17, UU12]. recognition [CXS10, EPH+15, HS12, Hsu14, ISP+10, LG14, OME16, OOK11].


[CSKH16]. sample [HRID16]. sampled [AST+16, CDM+15]. Sampling [AKN16, Yan16, BLKP12, BH15, CY09, CY13, CS17, DPNM11, DJ13, FM10, FBE11, FB14b, GFPSD17, GMO16, HH10, HDK+12, HTS15, HNS16, HS17, HDM+15, HCP15, IMK+16, ISK14, Ish10, KvdV14, KTO11, KB13c, LTT16, LC16, LL11, LM1+14, LZZ14, LAW+16, MZZ11, MCRL17, OL13, PBDW11, SEM12, SBN13a, SBN13b, STM+15, TJB12, YZ16, ZZ14, ZC14, DAB16].
Scalable [NLP+16]. scalar [Rod13]. Scale [XFG+16, ACD+13a, ACD+13b]. scales [GMPB12]. scaling [BG12, MA17, NPTS16, Pie14, RCM+13b, RR11, SS13a, VSA11, YN15].
SCC-DFTB/MM [RN17]. Scents [DR14]. Scerri [Sch10]. SCF [HNN+17]. SCH [ZL+10a]. Scheme
[SN16b, BG12, DK11, DGC14, HKR+14, ISN13, JSW10, MKO+13, MPBJ11, RK15, TCPPC14, UM13, WWD14, WDHZ13, YD17, dLC17, FPV13].

KVQC^11, KVR^10, KAG^12, LL^15, Lar^12, Lar^11, LWK^14, LJ^12, LC^17, LMZ^11a, LZ^14, LBPD^12, M^cvdV^13, MSC^10, MBR^15, MSvG^12, Mez^10, MMZW^14, MLCD^11, MCC^12, NPG^17, NFG^13, NDD^10, OYK^11, ON^14, R^11, RO^14a, RO^14b, RSR^12, RLS^13, SWM^10, SK^15b, SMRM^17, SJZ^15, SBvG^14, SA^15, G^15, TYNN^16, UT^11, UU^12, VRMR^17, Vor^12, WC^11, YAS^13, ZX^11, ZSS^13, ZKH^10, ZLL^13, dCLFGL^13].

Simulations [BRE^16, MFEM^16, RKDM^14, XFG^16, Aki^16, BM^12, BDTP^11, BW^15, BJ^15, BB^11b, BB^11c, BB^11i, CTR^13, CCOH^14, CVG^14, CLK^11, DG^11, DMN^14, DSD^11, DHF^11, DZT^11, DSK^17, DLZ^15, DDM^15, EK^15, FTW^12, GBL^11, GR^11, GCW^14, GP^11b, Has^14, HFSO^12, HPSK^12, HDPM^14, HYUS^11, HJ^10, HHWL^17, IPAA^11, JIS^13, JWO^15, JMS^14, KV^13, KCK^15, KvdV^14, KGHK^12, KGHC^15, KLOS^10, KTO^11, KSR^16, KSWL^16, KWL^16, KV^15a, KPF^15, LH^11, LRvdSM^15, LZ^12, LPS^13, LMI^14, LZLMP^16, LAS^14, MN^15, MCRL^17, MTvG^12, MFEM^15, MADWB^11, MK^17, MB^14, NST^14, NF^13, NNK^16, NTNY^15, Oht^16, OCL^11, OLY^17, OZ^14, OC^15, P^15, PH^17, PZCL^16, PL^14, PM^13, PS^13, PS^10, PNG^10, Rd^12, RLG^11, RSR^15, SBV^10, SS^13b, SBT^17, SIK^10, SJ^17].

simulations [SMP^17, SYN^12, SK^13, SB^15, SWB^12, SDMS^13, SV^11, VSA^11, VKTR^15, VM^11, WKLC^12, WH^11, WWKS^11, WLC^12, WBF^17, WG^14, WC^14, XFG^15, XWSW^13, YKO^11, YSG^12, Yon^16, YHVM^12, ZZY^16, ZDKM^12].


LHKS12, LH14b, MSS+13, MBE16, MBRC16, MPBJ11, NHH16, RLL+10, RS13, SG13, STS15, VT14, WF16, WTH+16, XML+15, XMSZ16, ZCGM11]. **small-molecule** [ETLS17, WF16]. **smaller** [MCK17b]. **smallest** [PMT16]. **SMD** [ALK+15]. **smeared** [ENKK+17]. **SMILES** [TTB+10]. **SMILES-based** [TTB+10]. **Smoluchowski** [SG10a]. **smooth** [AG11, EFS16, JLCA17, ZSB+16]. **smoothened** [MCK17b, PMG+16, RDT14, YW12, ASS10, PKK17]. **Sn** [MCK17b, PMG+16, RDT14, YW12, ASS10, PKK17]. **SnCl** [dSDdAR10]. **SnO** [DHE+12]. **Sodium** [KLN16]. **Soft** [SJC11, Ben17, BG12]. **Software** [RLLHL12, RNSF+16, Ras17, Rez16, RR14, RdA12, RSR+12, RCM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sie15, SJ17, SWB+12, SDMS13, TNYN16, TSC+13, TTR+12, TTL+12, UU12, VMRSH+17, VVV+15b, VAR12, VBV13b, WdVN12, WDY13, WPM+15, WF16, Wei12b, WHK+12, WHJH13, WG14, WCJ+14, XML+15, XYX17, YWJ+16, YZZ16, Yes12, Yes15, YHH+13, ZDKM12, ZLL+13, dVAG16, CCC+11, DBF14, MSvG12, MJG+15, SBV10, SGM+13, Yap11, ZCS+15, She12]. **softwares** [All11]. **solar** [ACS12, DGL+13, JYS+12, LZZ15a, SLC+15, TZ12, VAA14, YJN+11]. **Solid** [RSK+15, ASS10, CL16, HLS12, HBI+17, KLN12, POB13]. **Solid-state** [RSK+15, HBI+17, KLN12, POB13]. **solids** [BK11, HAI+16, MDT13, MS15, dLRL11, Pon11, SN16a]. **solubility** [KKO+16]. **solute** [BRLS08, BRLS12, EOA+11, TKT11, YKO+11, Yan11]. **solutes** [GC11, PAK15]. **solution** [AvKSP16, AK10, DR11, DBM+17, DP15, EOA+11, GAI13, GAI14, HDK+12, HAL14, HNN+17, KTN10, KVR10, LVC10, MMB+17, MFN+12, PMC+17, PGW+17, SJWE10, TKNN10, UCFR16, WLB+10, WC13, XTG+11, ZLL+10, ZZO+11, vADC+14]. **solutions** [Ber17, CFC15, EK15, Kri0, OCW+15, SM14a]. **Solvation** [RNSF+16, ZBP11, CGB16, FGM11, GMMH+16, GPK12, HRC13, JMLL13, JGS+17, Jor17, MS15, MBE16, NW17, OBU12, PL14, RK16a, RK16b, SL14a, SK12, SY11, SMM15a, SMM15b, TCC+13, WXL17, YOMT14, YAS13, Yan14, ZCS+15]. **solvation-free-energy** [SMM15a, SMM15b]. **solvational** [FCL+10]. **Solvatochromic** [MKH15].
solve [PNW+16]. Solvent [KC13b, AKK+16, BEM14, BRLS08, BRLS12, CAD16, CBG16, EK15, FZy+12, FD16, HDL+17, Ha14, HYUS11, KJDB12, KB11b, KCPMG12, LH+10, LC17, LzL+16, LWZ+17, MBC11, MBC13, MS11, ML14, MCG15, MCC12, MNNK10a, MNNK10b, PDMT10, PS13, RdA12, RK16, SLT14, SBV10, SK17, SLX+15, SYH12, SCMA+17, SKMS13, TYN15, WWKS11, WXL+12, WBF17, YOMT14, Yan14, YJ11, BK17a].


Solving [KV13, SG10a, BYE+16, GA14, SK15a]. solvolysis [OSS10].

SOMA [BMFG16]. Some [RCM+13b, CME11, CCYL11, CXS10, MJLV14b, MJLV14c, Vyb16, ZPF10].

sometimes [VDVR14]. Song [JW12]. Soon [Ano16-75, Ano16-80, Ano16-81, Ano16-82, Ano16-83, Ano16-84, Ano16-85, Ano16-86, Ano16-87, Ano16-88, Ano16-76, Ano16-77, Ano16-78, Ano16-79].

soot [KAR12]. SOP [AKK+16]. SOP-GPU [AKK+16]. Sorafenib [GMASBF16]. Sorting [NMF+14]. Source [TCB16, Aki16, APK14, BZH14, CD13, FBY+17, HLS+13, KSD+12, PHT17, SMRM+17, XTC+11, Yap11, Yes12]. sources [BK13]. Space [vRWS17, ACD+13a, AD10, Cas13, CH16, CXS10, DK11, GA14, Gk15b, Hb14, HP10b, HSB+11, JCGVPH17, LMZ11a, LLF16, LAW+16, MBFP15, PDG+16, SS13a, SHL+11, SCW13, TJB12, WDHZ13, YD17].


specificity [LJW+11b, LBS10, ZX11]. Spectra [PAK14, AMQ+14, FD13, FF11, GWF11, GGM+12, GZ12, HRH+17, KASH14, Kow11, LBC+12, LX11, MAK+14, MCLD10, NHF+10, PMC+17, PD10, DCOD13, PDG+16, RJS17, SGDT10, SB15, SR11, TYN15, TG12b, Tsi14, WGL12, WW14]. spectral [Ano15-58, BH14, HRMAL+13, KZ16, NS14, QZM11, RG1L11, SFDE16].


structured [GEP+14]. Structures

[DLT17, SNS16, BHNS14, BPI5, Ber17, CL16, CCOH14, CV12, DVVP14, DH14, DZA11, GS12, GSS13, HS+11, HTS17, HS12, Hua16, IYK11, KNE11a, KOT11, KOT13, KDT+12, KSW16, LABSG17, uLhY11, LXZ+10, LLSW14, Lüc14, MCS11, MTKM14, MPA10, MPA12, MP13, Mr14, MH10, MCA15, MP17, PRP15, PW+16, QM11, RHRCH16, Raol11, RCR+16, RvL11, RHJ11, RvK13, SFR+10, SWA13, SFR+11, SJD11, SKY+11, TN10, TFQ+10, TFQ+11, UCFS16, WKC11, WD10, YNH+17, ZSL+11, ZLY+16, ZP13, CMD13, PGCT+12]. studied [Ish10, KRTB10, OLY17, RHPWS13, RI10, TS15b].

Studies [JW12, AALCM11, BLS10, BRGN12, BLG10, DMN15, BIL10, DXL+10, GZZM16, GEP+14, JLS+10, KG15, KP11, LCWW10, LJL+11, LWD13, RCM+13b, SB10, SLHW09, TDP+12, VSD10, WCAH10, YKH+10, YPC+10, YDL+10, ZSL+12, ZSL+10a, ZYG+15, ZX11]. Study [JLH+14, VL17b, AS11, AS15a, AAMA+11, ASMS10, ANH+11, APA+14, APY+16, ALH+10, BEM14, BE14, BHB+17, BEEL14, BSJ12, BLG11, BRLS08, BRLS12, BL12, BSL11, CCLP12, CCCLRO14, CWHH11, CCJ+11, CKL+11, CXW14, CBTZ16, CL16, CC14, Chu10, CG12, CB1c, CPL11, CB1d, DAS15, DR11, DI11, DLSD13, DXS+11, EO+11, EV14, FCL+10, FF11, FCD10, FBEM11, FL15, FB14b, GA14, GG10, GYX+10, GVP+10, GD10, GTK10, GWZ15, GNGCA10, GGM+12, HKR13, GPS11, HZ11, HDB15, HRL11, HBR17, HVS16, IL11, II1F+10, IN13, IIHY15, II10, JA10, JS17a, JCG+10, JAH+17, JJAB16, JW16, JYS+12, KD10, KKPT11, KOP+14, KC13b, KB13, KT12, KG11, KN16, KS13b, KP10, LC10, LY10, uLhY11, LP11a, LL13a, LLL+10, LD10, LSL+10, LCL+10, LZ+11, LZH11, LWL+11]. study [Li14a, Li14b, LGW12, LT13, LJW+11b, LBTV11, LBTV12, LTP11, LYSS11, LH12, LH14b, LLSW14, LWXC16, LHT15, Lu11, LJG+11, LPTM17, MMS16, MC10, MG15, MCF10, MJL14b, MAPB12, MF+12, MH11, MWJ+11, MS11, MPS13, MHRR11, MBRC16, MO17, Mor15, MIS+15, NHE+10, NASH15, NC12, NC13, NC14, NJX+10, NFI+16, OPR16, ORZ11, OSS10, OSHG17, OME16, OOK11, PVL+13, PGCT+12, PP10, PGC12, PSG+15, PH12, PAK17, PPH+10, QYL10, QZ10b, RAGL11, RAR+11, Ray13, RS13, RS14, RVV+13, RSLM12, RKG11, RSKG14, SN16a, SSP+13, SGDT10, SJD14, SCM+15, SRF+17, SVM10, SNS16, SGS+16, SE14, SCMA+17, Su10, SKY+11, STS+10, SKTT11, SZS16, STS15, SGHL13, SIG+15, TM16, TLA10, TSR+16, TLR16, VKNT16, VPR10, VAR12, Vik11, VLGK+17, VED10, WKC10a, WLC10, WDLG12, WLHZ12, WYL+15, WMN17, WXH+10]. study [WD10, WMW+10, WZQW10, WS11, WHDL11, WCL+11, WYGW12, WDP+12, XDL+10, XZ11, XWW+11, YZGS14a, YZWC11, YHG+11, YZ13, YR13, YJZX13, YLZ+10, YKH15, YSRR10, YCGA10, YB11, YY12, YZ15b, ZCK+16, ZWGO16, ZTH+15, ZPP+16, ZXS+10, ZZZ+10b, ZZWT12, ZYLL12, ZLLL12, ZSZ+14, ZDX11, ZWY+10b, ZWY+10a, ZBP11,
Symmetrizer [LPS12]. Symmetry
[CAA10, EP15, VVV+15a, BV14, CWZB10, DZA11, Dry14, FF11, HB14,
KTT16, KC13b, NDD+10, PBZA13, Sch13, VGT16, YKH15].
symmetry-adapted [FF11, YKH15], symmetry-invariant [CWZB10],
synchronicity [dSVdM+16], synthase [AALCM11, SYH12, XLY10].
synthase-catalyzed [XLY10], synthesis [ZZWT12], synthetase [LBS10].
syringe [ZWS+10]. system [BEEL14, BTT10, BCCO10, CS14, CJZS10,
GRS15, HSY+11, HDM+15, LL11, LYL6, LZY12b, MLZZ12, NTNY15,
NSP15, RHT+15, SZBM13, TL16, VBDS+11, WLF11]. Systematic
[GP11b, ML14, SA13, SCMA+17, UT15, VLGK+17, AIGP15, BEL+11,
FM10, Ish12, LG11, Pet11, STS15, VVGL17, WG12, RFHG10]. Systems
[RMM16, AST+16, APK14, BV14, BYV+12, BK13, BG13, CSS17, CEBO15,
CKL+11, CLK11, EP12, GG10, Gar12, GP12, GBW+14, GR10b, GWX12,
HS11, HCD+10, HvM16, ITIN15, JSXH16, JS17b, KV12, KGM12, LBG16,
LCPS13, LPLA13, MSC+10, MG14, MOS12, MS12, NYN17, NCV10,
NFG+13, NO16, NKK+16, NS17, OPB+12, OC14, PAK17, PAT+10, PBBP11,
PD12, RJPB12, RVCF13, SCQJ13, Sch12, Sea10, SWB+12, SG13, TSN16,
TCX+13, UT15, WCY+11, WWU12, WS11, YCK16, ZSB+11, ZT14, HvM17].
T [BB1+11, CSGOA17, Gil11, MLCD11, OP16, SRR16, YJ17, BBG+11,
BH13, CGBK13, HLS+13, Sch13]. T-cell [CGBK13]. Table
[Ano16-115, Ano16-121, Ano16-122, Ano16-123, Ano16-124, Ano16-125,
Ano16-126, Ano16-127, Ano16-128, Ano16-116, Ano16-117, Ano16-118,
Ano16-119, Ano16-120, Sce07, Sch10, AAC+16, Fom11, JMS13, MGS+16].
tables [BDdS13, LZ12]. TaBoo [HTS15]. tabu [GBSE11].
tabu-search-based [GBSE11]. tabulated [LL10a]. tail [MBC13]. tailoring
[RKGN10]. tails [GSD10]. Taming [CCM15]. tar [HCD+10]. tar-MD
[HCD+10]. target [FMG12]. TargetATPsite [YHH+13]. targets
[BK13, MPBJ11]. Task [CSSB11, HPSK12, KG13]. task-oriented [KG13].
[WHJH13]. tautomeric [SJWIE10]. tautomerism [BMB13, LGOM+15].
tautomerization [BH13, BZH14]. tautomers [BZH14, dALdS+15]. Tb
[SRL+15]. TD [CCB15, CH10, EFAC13, HRJ+14, HRJ+15, JRSH14,
KLK+13, KP10, LZL+10, LZHH11, LSH+11, LYSS11, RDF+11, SRF+17].
TD-DFT [CCB15, CH10, EFAC13, HRJ+15, JRSH14, KLK+13, KP10,
LZH11, LYSS11, RDF+11, SRF+17]. TD-DFT- [LSH+11]. TD-HF-based
[LSH+11]. TDDFT [SFCCK+15, LRBB12, QCR12, SFCCK+14]. Te
[SPL+12]. technique [AMGB10, LZZ+13, TSR+16]. techniques
[BCP+10, BCG10, GVP+10, SDF+17, SY11, WBN+13]. tellurium
[RRK16, ZWGO16]. Temperature
[KKO+16, LPE+10, LTLC12, PBE16, SY16b, CH16, DKT13, DLSD13, LL11,
OGL10, TLG+12, TM16, VED10, WMW11, YW12, OCW+15].
temperatures [NMLD13, RHNN10]. tempering
[LAW+16, MO15, MO17, NPTS16, TKT11]. Template
[Mau14, GLF16, ME10, YHH+13]. Template-free [Mau14, YHH+13].
tension [NFPD13]. tensor [Elk16, EWK+13, GMBX+16, HXM+16,
JMX+16, KK17a, NFPD13, NIT15, NFI+16, TKC+11, XFX+16]. tensors
[EPD+11, PKH14]. terahertz [KB16], term [DSF17, JBSQG11]. terminal
[IMK+16]. terminally [KLS10, KML10]. terminally-blocked
[KLS10, KML10]. terms [BAS14, CZY11, CWZB10, RRH12]. ternary
[RDT14]. tertiary [OPR16, SM11]. tessellation [MOS12]. Test
[PHC13, BS10b, DPOS16]. tested [HMM10]. Testing
[Gil11, RLD12, JGS+17]. tests [Aon15-59, CNK97, ENKK+17]. tethered
[CZA11]. tetra [WDLG12]. tetraamines [SB10]. tetracarboxylates
[CRC13]. tetracoordinate [XHz15, ZYW+16, ZLY+16]. tetracene
[ABDG12]. tetrramer [Ish10]. tetramers [LYL16, SZS16]. Tetraoxide
[JW12, SLHW09]. tetraprotonated [ZWY+10b]. tetraradical
[Cas14, YSSB12]. tetrasaccharide [NPG17]. tetraflafulvalene [MCF10].
Tetrazine [JW12, MCA+16, SLHW09]. Tetrazino [JW12, SLHW09].
Tetrazino-Tetrazine-Tetraoxide [JW12, SLHW09]. tetrel [YKH15].
TF [XMSZ16]. Th [MCK17a]. their
[ARRC15, Aon11, CCI2a, CBTZ16, CFC15, CB11a, DLT17, DSM+11, HJ13,
JML13, JHMB+09, JHMB+11, KG15, KNE11a, KRSC12, SBR13, TN12,
Tak11, TY10, TS11, VV15, VVBL17, XDL+10, ZYW+10a]. them
[WCWV15]. theorem [CDB10, KSH13, YB16, ZM11]. theoretic
[MCC12, ZLW10]. Theoretical
[AvKSP16, AMA+11, BHB+17, BSDP16, CWT+12, DBM+17, DGL+13,
FF11, GYX+10, GLZ17, GLM+17, HDHL15c, JW12, KCB+12, KS13b,
LCL+10, LWL+11, LLW12, LZY+12a, LWWG12, LWXC16, LGJ+11, MLQ+12,
MSV16, NFT+16, OSS10, OAN15b, PKK17, PM13, PE11, RS17, SB10,
SKY+11, STH+10, SZS16, SLC+17, SGHL13, TPL+10, WMW11, WHDL11,
WCL+11, WS12, YJN+11, YPC+10, YHG+11, YCAG10, YYT12, YGDZ15,
ZBL+10b, ZZL+10a, ZYL+12, ZLLL12, ZSZ+14, ZYG+15, ZBMDH15, BLS10,
BE16, CHZ12, CKL+11, CBTZ16, EV14, GG10, HDM15, HHPH14, LWW+12,
LDD17, LZW+11, MPSS11, NHF+10, NJX+10, PH12, PSSdP10, Pog10,
PH10b, RZG+13, RVCF13, RVP+11, SSF+13, SJ11, SLHW09, SKT11,
SHG+16, Tak11, TL16, WSH10, WZQW10, YK13, YZCW11, YZ13, YB11,
Zhai12b, dSAdSL13, HDHL15a, HDHL15b, KZK+12, TDP+12]. theories
[OM12, WCWV15]. Theory
[IUK+11, SXZ13a, SXZ13b, WM12, AMK11, ALK+15, AR10, ARAG17,
ABDGN12, AG12, ASS10, BY11, BLBG+13, BZB+13, BG13, CHG+16,
CSAdOM17, CWHH11, CCM15, CF14, CC11, DCHL12, FRSA14, FD16,
GHL17, GZL+12, GCM15, CY10, GNGCA10, GND+12, GEG11, GPK12,
Han11, Hll13, HNN+17, HRJ+14, HRJ+15, HG10, ISN13, IKN13, JRSHP14,
JLH+14, JW16, JYS+12, KHWB17, KL12, KM13, LC12, LBG16,
LCL+10, LLH17, LPMT17, MCC11, MAK+14, MWJ+11, ME10, NMDL13,
NO16, Niz13, ORZ11, OZLSB12, PAK17, PML+12, PPH+14, Pie14, Pyy13,
translationally [MRO17], translocation [MJC14]. transmembrane [DSF17, LMI+14, LAW+16, WXL+12]. transmission [LLJ12].

transphosphorylation [WXY14]. Transport [DJX+11a, DMN15, CWHH11, CBTZ16, DMN14, DJX+11b, HLWD15, LHO17, LJ+12, NS17, PGY15, SLIB12, SY16b, TCX+13, ZYG+15].

transportation [LZY+12]. trapped [DM15, VIT+15, WXL+12]. Treating [JLCA17, SMP17]. Treatment [HSH15, CSGOA17, GPK12, Has14, HGHP14, MG14, NS10, Sch12, SSWX14].


triads [YKH+10]. traminoguanidinium [ZYL+10].

triangles [She12]. triangular [TS11]. triangularly [LWZK13].

triangulenes [GSM15]. triarylamine [KGR+16]. triazine [WDLG12].

triazines [YPC+10]. triazol [ZZWT12].


triarylamine [KGR+16]. triazine [WDLG12].

triazines [YPC+10]. triazol [ZZWT12].


triangulenes [GSM15]. triarylamine [KGR13]. triazine [WDLG12].

triazines [YPC+10]. triazol [ZZWT12].


triangulenes [GSM15]. triarylamine [KGR13]. triazine [WDLG12].

triazines [YPC+10]. triazol [ZZWT12].


triangulenes [GSM15]. triarylamine [KGR13]. triazine [WDLG12].

triazines [YPC+10]. triazol [ZZWT12].


triangulenes [GSM15]. triarylamine [KGR13]. triazine [WDLG12].

triazines [YPC+10]. triazol [ZZWT12].


triangulenes [GSM15]. triarylamine [KGR13]. triazine [WDLG12].

triazines [YPC+10]. triazol [ZZWT12].


triangulenes [GSM15]. triarylamine [KGR13]. triazine [WDLG12].

triazines [YPC+10]. triazol [ZZWT12].


triangulenes [GSM15]. triarylamine [KGR13]. triazine [WDLG12].

triazines [YPC+10]. triazol [ZZWT12].

100

[BM12, BE16, CRC13, CB11c, Dil15, HLWD15, JYC+16, LH14a, MY17a, MY17b, MKH15, RKB+14, SZX13a, SZX13b, VED10, WvRSM14, ZX11].
type-II [CB11c]. types [SKY+11, UT15]. typical [TZ12]. typing
[FP17b, YPKB12].

U [MCK17a, RKB+14], Ubbelohde [KTT16]. ubiquitin [MO17]. UCCSD
Umbrella [DAB16, FB14b, AKN16, HH10, HDM+15, Ish10, KTO11, 
LMt+14, OL13, ZZ14]. unbiased [ISO+13]. uncertainty [Fer17, Han11].
unconventional [LDJ+10]. underlying [RN17, SGPS+17].
Understanding [DLZ15, Lun12, RCM+13a, TZ11, dCDP15, BH13,
FCOGM12, KNE11a, LGVA14, VVJ15, ZX11]. unexpected [HYYZ13].
Unexpectedly [SDF12]. unfavorable [PRP15]. Unified
[PPUBGD10, CVT+11, TNYN16]. uniform [TH13, YWJ+16].
unimolecular [AMAA+11, STM17]. union [KRSC12]. unique
[GS11, uLhY11]. unit
[CKKK16, DZA11, DGLt+13, EP10, Elk16, PMT16, SRLt+15, WS13].
unit-based [WS13]. Unitary [SSSM15]. united [JGS+17, Jor17, ST11].
united-atom [JGS+17, Jor17, ST11]. units
[CCCLCGRO14, CY11+10, FCOGM12, GBL+11, HASR+12, HEMCZE+14,
WSGN11, YWJ+16, YN15, ZKE+17]. universal
[AH10, AJR16, Gar12, SYN+12]. unknown [GPdC+16, KYN+17, MFR10].
unperturbed [Gri13]. unraveling [HYYZ13]. UNRES
[KMLS10, Sie15, SJ17]. unrestricted [BW11a]. Unsaturated
[HPT16a, Tsi17]. unsulfated [SA10]. unoctium [TH13]. unusual
[KYCL11, LJJ+11]. unzipping [SM15, SM16b]. Update
[CZAF17, MRO17, DPNM11]. updated [BCJC+14]. Updates
[AIGP15, Ak16, APK14, AAC+16, BTA+13, BHB12, BSCSJ+13, BSZ+12,
Ber17, BJ15, DMN15, BFH+13, CB14, CSEMB+16, CZAF17, CAT+13,
DJ12, DVVP14, DDK14, DWC17, DSK17, ESBI3, EWK+13, FN12,
FSCc+14, GMSdG15, Gar12, GJMPAM+14, GLW13b, GS12, GCP+13,
GCC14, GBWc+14, GH16b, HLS+13, HRB+17, HDH12, HPT+16b, HPSK12,
HHCT+13b, HH16b, HG13, HYMIZ6, HKR+14, HL14, HC14, IGK16, JH+13,
JWW+14, JLCA17, JP15, KS13a, KS15, KK17a, Kan15, KB16, KL+17,
KDTc+12, Kos16, KG13, KWL+16, KK17b, KGW15, KYG+15, KAG+12,
KSW16, KPF+15, LPS12, LJ+12, LS12, Leh15, LRvdSM15, LDB+17,
LLZZ12, LBB+15, LWZ+17, LC12, LAS+14, MDTD16, MBR+15, MB14,
MB16, NKJ16, OV14, OPB+12, OZS+13, OC14, PSS14, PGL+15, DBDP16,
PW12, PPM15, PPH+12, PVZ13, PG14, RLLHL12, RNSF+16, Ras17].
Updates [Rez16, RR14, RdA12, RSR+12, RCM+13b, SM14a, SFGc+17,
SK15b, SWA13, SMRM+17, She12, SC15, Sie15, SJ17, SWB+12, SDMS13,
TNYN16, TSc+13, TTR+12, TTL+12, UU12, VMRS+17, VV+15b,
VAR12, VB13b, WdVN12, WDJ13, WPM+15, WF16, Wei12b, WHK+12,
WHJ13, WGU14, WCJ+14, XML+15, XYX17, YWJ+16, YZZ16, Yes12,
Yes15, YHH\(^+13\), ZDKM12, ZLL\(^+13\), dVAG16, KKR\(^+13\)]. updating [UM13].
upgrade [ZSLL17]. uptake [WKC10a]. uracil
[HvM12, LGOM\(^+15\), LJW11a]. uracil/uracil [HvM12]. uranium [OSS10].
uranyl [OSS10]. URBOMOLE [BBG\(^+11\)]. ureas [FCL\(^+10\)]. uracil
[SPP\(^+13\)]. ureido-benzenesulfonamide [SSP\(^+13\)]. uridines [DSP16].
urokinase [BM12]. uroporphyrinogen [BEL\(^+11\)]. uroporphyrinogen-III
[BEL\(^+11\)]. Use [DCOD13, HCD\(^+10\), MPA12, MMZW14, NPTS16, NC14,
NDD\(^+10\), RLD12, WM17, Yes12, BCP\(^+10\)]. used
[PGY15, Pie14, PLAG11, TH13]. useful [SMGB11]. usefulness [PSP15].
user [All11, DBF14, HH16b, JJW\(^+14\), LBB\(^+15\)]. user-friendly
[SFR\(^+11\)]. users [GKV\(^+13\)]. uses
[BCJC\(^+14\), FHMB15]. Using
[BS15, Car14, DLL\(^+10\), HH10, HPSK12, LLvG10, LG14, MP11, QLQ11,
SK17, TNG\(^+10\), WF16, AG11, AGM\(^+13\), AC12, BW11b, BMRI11, BDTP11,
BB11a, CVT\(^+11\), CSSB11, DWL11, DBK17, DFF\(^+15\), DCHL12, DLZ15,
EWK\(^+13\), FF11, FLM11, FL15, Gar12, GRS15, GFPS17, GMO16, GZM11,
GRL\(^+11\), GRL\(^+12\), GMBX\(^+16\), HASR\(^+12\), HNS16, HLW\(^+17\), HDL\(^+17\),
Höf14, HBL12, HYUS11, HJKJ13, HZSS17, HHWL17, Hug14, HRH\(^+17\),
Ish10, IH\(^+13\), JLH\(^+14\), JMS13, KV13, Kan15, KERY\(^+16\), KT10, KLOS10,
KTNN10, KP11, LBSIS16, LPK16, LRvdSM15, LZ12, LCH10, LCL\(^+10\),
LMR14, LHG11, LTA\(^+11\), LBDP12, MS17, MZZ11, MRB14, MJJC14, MN15,
MY17a, MSS\(^+13\), MKM\(^+17\), MCUJ15, MVKS10, MBA\(^+13\), MFR\(^+17\),
MOIM13, MMJ10, MS15, NLP\(^+16\), NASH15, NHN16, OCW\(^+15\), PGdO\(^+16\),
PC11, PG15, Pie14, PJ13, RB13a, RLDJ17, RDDS10, RHIJ11, RS13]. using
[RRK14, Ric16, REL17, REV\(^+17\), Rui11, RFHG10, REH13, SHMO11,
SMF14, SDF\(^+17\), SBV10, SA13, SCW11, SEF\(^+16\), SHT\(^+11\), SKKS13, SY11,
SRS14, SSZS16, STS15, TYZ\(^+16\), Tak14, TKNN10, Tsi17, TJB12, UTM11,
VKAM12, VECT12, VI17, WKLC12, WdVN12, WLC12, WZ17, WJX\(^+10\),
WDHZ13, XTY\(^+14\), XYX17, XWW\(^+11\), YWJ\(^+16\), Yon16, YN15, YDX16,
ZWLX11, ZLI11, ZLT13, ZWS\(^+10\), ZP13, ZH12, ZHHX11, dLC17, LHL\(^+10\)].
utility [YHV12]. utilizing [BVY\(^+12\)]. UV
[GGM\(^+12\), KASH14, RDF\(^+11\), RVdMB16]. UV-photoexcitation
[RVdMB16]. UV/Vis [GGM\(^+12\)].

V [WWKS16, LZL\(^+15b\), MG11, PBE16, WRM\(^+12\), WYGW12]. valence
[FF11]. Valence [WM12, YWZ14, BEEL14, BACSCJ\(^+10\), FE14, GCW16,
Hil13, HAI\(^+16\), KGR\(^+16\), LLW12, LWW12, POB13, RHRCH16, RVL11,
SSMW09, SCSW13, TM16, WWU12, XP13, XhD15, vLBBR12, GWF11].
validation
[GMMH\(^+16\), GCP\(^+13\), PFVL14, WMW\(^+10\), ZSTI14, GMG\(^+10\), HM13].
validity [LP11b]. value [SG10a]. values
[BA11, GK15a, SK12, Zha12b, Zha12a]. vanadia [GNGCA10]. vanadium
[WYGW12]. vapor [BDTP11, SISK10]. variable [KDB13]. variant
[TKT11]. variants [SLY\(^+10\)]. Variation [IMK\(^+16\), LvG13a, MTvG12].

Volume

Waals
[BLF14, BB11a, BC13, CR14, DS12b, DSF17, KBC12, KCK+15, KGHK12, KLN12, LCH+15, SMGB11, SLIB12, SJZ+15, SYZ+17, YZZ+17, ZY14].
REFERENCES

[FLM11, LLBO12, LSHH12, PDG+16, WWD14, XML+15]. X10 [LMR14].


Xe [SKMS13, BBI+11, MLGB16, SKMS13]. XH [UT15, CCCLCGRO14].

Xiaobo [Ano12u]. Xiaojian [Ano12u]. Xinli [JW12]. XML [LDB+17]. XO

[GWZX12]. XPS [IN13]. XQDPT2 [KKL+13]. XY [CXS10]. XYG3

[SZX13a, SZX13b, ZWLX11].

Ye [SKMS13, BBI+11, MLGB16, SKMS13]. Yeast [ZZY+16]. YH


Yy-DNA [ZLL+10].

Z [JJJ16, FCOGM12, JJJ16]. Zebularine [SCW11]. Zeolite [SN16a]. Zeoe-

lites [LZTV10, Lar11, SN15, SDB+16]. Zero [Pol13, Tac17, VED10]. Zeo-


SPS+12, YSSB12]. Zintl [RDT14]. Zn [SLIB12, GPdC+16, QLYL10, RRF11,

XP13]. Zn-metalloenzyme [GPdC+16]. ZnH [HYD10]. ZnO [HSH15, VI17].

ZnPh [RDT14]. Zns [NNS15]. ZnSe [Lar12]. ZnX [SPS+12]. Zone [PBE16,

BPE16]. Zone-folding [PBE16, BPE16]. Zones [TDKT10]. Zora [ARAG17]

[JKS+16]. Zr [MCK17a, YW12, TCPCC14]. ZrN [FAA15]. ZrO [RRC+15].

ZrS [BE14, BPE16]. ZSM [Mor15, Pon10]. Zwitterion [DQ16, ZZWT12]

.Zwitterions [PVS12].

References

[AAC+16] Francesco Aquilante, Jochen Autschbach, Rebecca K. Carl-

son, Liviu F. Chibotaru, Mickaël G. Delcey, Luca De Vico, Ignacio Fdez.

Galván, Nicolas Ferré, Luis Manuel Frutos, Laura Gagliardi, Marco Garavelli, Angelo Giussani, Chad E. Hoyer,

Giovanni Li Manni, Hans Lischka, Dongxia Ma, Per Åke Malmqvist, Thomas Müller, Artur Nenov, Massimo Olivucci,

Thomas Bondo Pedersen, Daoling Peng, Felix Plasser, Ben Pritchard, Markus Reihner, Ivan Rivalta, Igor Schapiro, Javier

Segarra-Martí, Michael Stenrup, Donald G. Truhlar, Liviu Ungur, Alessio Valentini, Steven Vancoillie, Valera Verya-

zov, Victor P. Vysotskiy, Oliver Weingart, Felipe Zapata, and Roland Lindh. Software news and updates: Molcas 8: New

capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational

Abdel-Azeim:2011:ZHB


Altarawneh:2011:RCH


Abolfath:2010:DBR


Arthur:2016:EIC


Arthur:2016:PIG


[ACD+13b] Kalipada Adhikari, Sudip Chattopadhyay, Barin Kumar De, Amitava Sharma, Ranendu Kumar Nath, and Dhiman Sinha.

**Asaduzzaman:2012:RBD**


**Affentranger:2010:PFC**


**Aquilante:2010:MNG**


**Anacker:2014:NAB**


**Addicoat:2013:SSD**

Matthew A. Addicoat, Syou Fukuoka, Alister J. Page, and Stephan Irle. Stochastic structure determination for confor-

Anand:2016:HBA


Abraham:2011:OPM


Antony:2012:FIP


Anthopoulos:2013:GAM


Astray:2013:EFP


Artemova:2011:CNS

Svetlana Artemova, Sergei Grudinin, and Stephane Redon. A comparison of neighbor search algorithms for large rigid

**Artemova:2011:FCA**


**Alonso:2010:USA**


**Afanasyeva:2015:SNU**


**Artemova:2016:AMS**


**Aono:2010:PTP**


**Akimov:2016:SNU**


Aidas:2015:AAP

Allouche:2011:GGU

Ai:2010:IBF

Allen:2010:EAM

Al-Muhtaseb:2011:TSU
Aguilar-Mogas:2010:IAB


Addicoat:2011:DFT


Alberto:2014:ESI


Aquino:2011:CTS


Anonymous:2010:CFE


Anonymous:2010:JCC

REFERENCES

Anonymous:2011:TAT


Anonymous:2012:CIIa


Anonymous:2012:CIIb


Anonymous:2012:CIIc


Anonymous:2012:CIIId


Anonymous:2012:CIIe


Anonymous:2012:CIIf

REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES

Anonymous:2013:CIiab


Anonymous:2013:CIiac


Anonymous:2013:CIiad


Anonymous:2013:CIiac


Anonymous:2013:CIiab


Anonymous:2013:CIiab


Anonymous:2013:CIiab

REFERENCES


Anonymous:2013:CIVk


Anonymous:2013:CIVl


Anonymous:2013:CIVm


Anonymous:2013:CIVn


Anonymous:2013:CIVo


Anonymous:2013:CIVp


Anonymous:2013:CIVq


Anonymous:2013:CIVr

Anonymous:2013:CIVs


Anonymous:2013:CIVb


Anonymous:2013:CIVt


Anonymous:2013:CIVu


Anonymous:2013:CIVv


Anonymous:2013:CIVw


Anonymous:2013:CIVx

Anonymous:2013:CIVy


Anonymous:2013:CIVz


Anonymous:2013:CIVaa


Anonymous:2013:CIVab


Anonymous:2013:CIVac


Anonymous:2013:CIVc


Anonymous:2013:CIVad

Anonymous:2013:CIVae


Anonymous:2013:CIVaf


Anonymous:2013:CIVag


Anonymous:2013:CIVd


Anonymous:2013:CIVe


Anonymous:2013:CIVf


Anonymous:2013:CIVg

Anon Anonymous:2013:CIVh

Anon Anonymous:2013:CIVi

Anon Anonymous:2014:CIIa

Anon Anonymous:2014:CIVa

Anon Anonymous:2014:CIVb

Anon Anonymous:2014:CIVx

Anon Anonymous:2014:CIVy
References

Anonymous:2014:CIVz


Anonymous:2014:CIVaa


Anonymous:2014:CIVab


Anonymous:2014:CIVac


Anonymous:2014:CIVad


Anonymous:2014:CIVae


Anonymous:2014:CIVah


Anonymous:2014:CIVai


Anonymous:2014:CIVaj


Anonymous:2014:CIVak


Anonymous:2014:CIVam


Anonymous:2014:CIVan


Anonymous:2014:CIVbi


Anonymous:2014:CIVbl


Anonymous:2014:CIVf


Anonymous:2014:CIVbp


Anonymous:2014:CIVbq


Anonymous:2014:CIVbr


Anonymous:2014:CIVbs

REFERENCES


Anonymous:2014:CIVn


Anonymous:2014:CIVo


Anonymous:2014:CIVq


Anonymous:2014:CIVr


Anonymous:2014:CIVs


Anonymous:2014:CIVt

Anonymous:2014:CIVu


Anonymous:2014:CIVv


Anonymous:2014:CIVw


Anonymous:2015:CIVa


Anonymous:2015:CIVb


Anonymous:2015:CIVu


Anonymous:2015:CIVv


Anonymous:2015:CIVw

Anonymous:2015:CIVx


Anonymous:2015:CIVy


Anonymous:2015:CIVz


Anonymous:2015:CIVaa


Anonymous:2015:CIVab


Anonymous:2015:CIVac


Anonymous:2015:CIVad

REFERENCES


Anonymous:2015:CIVam


Anonymous:2015:CIVc


Anonymous:2015:CIVd


Anonymous:2015:CIVe


Anonymous:2015:CIVan


Anonymous:2015:CIVao


Anonymous:2015:CIVap

REFERENCES


REFERENCES

Anonymous:2015:CIVax

Anonymous:2015:CIVay

Anonymous:2015:CIVf

Anonymous:2015:CIVg

Anonymous:2015:CIVaz

Anonymous:2015:CIVba

Anonymous:2015:CIVbb


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Anonymous:2015:CIVm


Anonymous:2015:CIVn


Anonymous:2015:CIVo


Anonymous:2015:CIVp


Anonymous:2015:CIVq


Anonymous:2015:CIVr

Anonymous:2015:CIVs


Anonymous:2015:CIVt


Anonymous:2015:ECS


Anonymous:2015:ECG


Anonymous:2015:OPS


Anonymous:2016:CIVa


Anonymous:2016:CIVb

Anonymous:2016:CIVc


Anonymous:2016:CIVv


Anonymous:2016:CIVw


Anonymous:2016:CIVx


Anonymous:2016:CIVy


Anonymous:2016:CIVz


Anonymous:2016:CIVaa


Anonymous:2016:CIVab

Anonymous:2016:CIVac


Anonymous:2016:CIVad


Anonymous:2016:CIVae


Anonymous:2016:CIVaf


Anonymous:2016:CIVag


Anonymous:2016:CIVah


Anonymous:2016:CIVai


Anonymous:2016:CIVaj

References


REFERENCES

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVaq


Anonymous:2016:CIVar


Anonymous:2016:CIVas


Anonymous:2016:CIVat


Anonymous:2016:CIVau


Anonymous:2016:CIVav


Anonymous:2016:CIVaw

REFERENCES


Anonymous:2016:CIVbc


Anonymous:2016:CIVh


Anonymous:2016:CIVi


Anonymous:2016:CIVj


Anonymous:2016:CIVk


Anonymous:2016:CIVl


Anonymous:2016:CIVm

Anonymous:2016:EPR


Anonymous:2016:IIa


Anonymous:2016:IIb


Anonymous:2016:IIc


Anonymous:2016:IIf


Anonymous:2016:IIg


Anonymous:2016:IIh


Anonymous:2016:IIi

REFERENCES


Anonymous:2016:IIR


Anonymous:2016:IIs


Anonymous:2016:IIt


Anonymous:2016:IICa


Anonymous:2016:IICs


Anonymous:2016:IICu


Anonymous:2016:IICw


Anonymous:2016:IICy

Anonymous:2016:IICaa

Anonymous:2016:IICc

Anonymous:2016:IICe

Anonymous:2016:IICg

Anonymous:2016:IICI

Anonymous:2016:IICK

Anonymous:2016:IICm
REFERENCES

15, 2016. CODEN JCCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES

15, 2016. CODEN JCCCHD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:ICab


Anonymous:2016:ICd


Anonymous:2016:ICf


Anonymous:2016:ICh


Anonymous:2016:ICj


Anonymous:2016:ICl


Anonymous:2016:ICn

2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


Anonymous:2016:IIEb


Anonymous:2016:IIEc


Anonymous:2016:IIEd


Anonymous:2016:IIEf


Anonymous:2016:IIEg


Anonymous:2016:IIEh


Anonymous:2016:IIEi

REFERENCES

April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Anonymous:2016:IIEa


Anonymous:2016:IIEe


Anonymous:2017:CIVa


Anonymous:2017:CIVj


Anonymous:2017:CIVk


Anonymous:2017:CIVl


Anonymous:2017:CIVm


Anonymous:2017:CIVf


Anonymous:2017:CIVg


Anonymous:2017:CIVh


Anonymous:2017:C IVi


Anonymous:2017:E


Anonymous:2017:IIa


Anonymous:2017:IIb


Anonymous:2017:IIc


REFERENCES

Anonymous:2017:II


Anonymous:2017:IIm


Anonymous:2017:IIn


Anonymous:2017:IIo


Anonymous:2017:IIp


Anonymous:2017:IIsn


Anonymous:2017:IIr


Anonymous:2017:IIIs

REFERENCES


REFERENCES


Manjaly J. Ajitha and Cherumuttathlu H. Suresh. Role of stereoelectronic features of imine and enamine in (S)-proline catalyzed Mannich reaction of acetaldehyde: an in silico

**Andersson:2014:PHE**


**Akbarzadeh:2015:HAA**


**Antila:2015:CTI**


**Alaghemandi:2011:CBT**


**Ansbacher:2010:CDM**

REFERENCES

Assadollahzadeh:2010:EPS


Abramyan:2016:CAM


Achazi:2016:TEI


Andoh:2017:EAP


Burger:2011:EPP


Bachler:2012:QCC

[Bac12] Vinzenz Bachler. A quantum chemical calculation on Fe(CO)\textsubscript{5} revealing the operation of the Dewar–Chatt–Duncanson
REFERENCES


REFERENCES


Bond:2010:FOS


Borrelli:2010:EHR


Baldov:2014:LEU


Bartolomei:2011:LRI


Borghini:2010:CRP

[BCP+10] Alice Borghini, Paolo Crotti, Daniele Pietra, Lucilla Favero, and Anna Maria Bianucci. Chemical reactivity predictions: Use of data mining techniques for analyzing regioselective azidolysis of epoxides. Journal of Computational Chemistry,


Bandura:2012:FPC


Bandura:2014:TZS


Bruckner:2016:TDC


Bendazzoli:2014:TPS


Brooks:2013:ENP


Bushnell:2011:FBP

REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES

Baranowska-Laczkowska:2013:PLR


Beker:2013:LCP


Baranowska-Laczkowska:2014:BSE


Baranowska-Laczkowska:2013:NBS


Berski:2010:IQC


Barbault:2012:IPB


Bhatia:2013:EDT


Borštnik:2011:DDF


Branduardi:2016:ARD


Barigye:2013:RFH

Balius:2011:IED


Boulougouris:2014:FEC


Bowman:2016:AMN


Bordogna:2011:PAP


Borkar:2013:HBC


Bandura:2016:AZF

REFERENCES


Bartolomei:2012:FDG


Bartolomei:2015:LES


Bandara:2017:ESS


Bello-Rivas:2016:STK


Beheshti:2012:HTO

Bondesson:2008:BSD


Bondesson:2012:EBS


Bosson:2012:IQC


Baranowska:2010:PBS


Black:2010:BHH


Brylinski:2010:QDL

REFERENCES

2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


[BSL*16] Daniel Bellinger, Volker Settels, Wenlan Liu, Reinhold F. Fink, and Bernd Engels. Influence of a polarizable surrounding on the electronically excited states of aggregated perylene...


REFERENCES

1054, April 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bertran:2010:IDN


Beruski:2014:ACD


Bultinck:2013:BFI


Bellafont:2017:PCL


Biswas:2012:SMS

REFERENCES


REFERENCES


[Chong:2016:ISC] Leebyn Chong, Fikret Aydin, and Meenakshi Dutt. Implicit solvent coarse-grained model of polyamidoamine dendrimers:

[CASANOVA:2013:PAM]


[CAMMI:2015:NEP]


[CANPEA:2010:SWM]


[CANPEA:2011:RCS]


[CARLSEN:2014:UOE]


[CASANOVA:2013:EIR]

[Cas13] David Casanova. Efficient implementation of restricted active space configuration interaction with the hole and particle

[Casanova:2014:HMT]


[Chilton:2013:SNU]


[Courcot:2011:MIB]


[Courcot:2011:OMMa]


[Courcot:2011:OMMb]

REFERENCEs


REFERENCES


REFERENCES

March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


**REFERENCES**

**Chattaopadhyay:2015:SSM**


**Chiang:2014:TBA**


**Chiu:2014:PAE**


**Cickovski:2010:MMD**


**Chiu:2011:DPI**


REFERENCES

August 2010. CODEN JCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


Chidthong:2010:ESP


Chong:2014:SDA


Chen:2016:WFE


Chang:2013:AAC


Cao:2016:HEI


Le Chang, Takeshi Ishikawa, Kazuo Kuwata, and Shoji Takada. Protein-specific force field derived from the frag-

Chen:2013:PPD


Condic-Jurkic:2010:CQM


Campen:2010:IES


Cvitkovic:2017:DME


Choi:2016:PHC

Chen:2011:RBS


Choi:2010:NAD


Chen:2016:NMA


Chakavorty:2016:ECB


Chung:2011:CST


Click:2011:QRN

REFERENCES


[CMD13]


[CPK12] Timothy H. Click, Sergei Y. Ponomarev, and George A. Kaminski. Importance of electrostatic polarizability in calu-


Cormanich:2016:IIC


Chen:2014:ESN


Cheron:2017:ESB


Carvalho-Silva:2017:DTS


Cardona-Serra:2016:SNU

REFERENCES


**Coe:2013:MCC**


**Carvalho:2013:PMD**


**Costanzi:2012:SSA**


**Chuev:2014:ESS**


**Chavent:2011:GAA**

Chai:2011:DFT


Cao:2012:TIP


Cui:2010:SRE


Chen:2010:AFE


Christodouleas:2010:TBE

Chen:2014:MRQ


Chen:2009:PRW


Chen:2013:EPR


Chen:2015:FFD


Chintapalli:2010:CLF


Cheron:2017:SNU

[CZAF17] Jean-Baptiste Chéron, Martin Zacharias, Serge Antonczak, and Sébastien Fiorucci. Software news and updates: Update

**Chandra:2012:TI**


**Curco:2011:SSA**


**Chen:2011:EMB**


**Dickson:2016:CFB**


**deAngulo:2012:RCA**

REFERENCES


[DBF14] José Diogo L. Dutra, Thiago D. Bispo, and Ricardo O. Freire. LUMPAC lanthanide luminescence software: Efficient and
REFERENCES


**Deshmukh:2011:IHB**


**Dickson:2017:OAS**


**Demichelis:2015:FPM**


**DiTommaso:2017:TAP**


**Drujon:2013:PHC**

deCourcy:2015:BOQ


Dong:2012:BCE


deCarvalho:2013:ICP


Pierre:2013:UIM


Dubaj:2015:IIM

REFERENCES


REFERENCES


REFERENCES


[DJX+11b] Zongling Ding, Jun Jiang, Huazhong Xing, Haibo Shu, Yan Huang, Xiaoshuang Chen, and Wei Lu. The finite-size effect on the transport properties in edge-modified graphene nanoribbon-based molecular devices. *Journal of Computa-
REFERENCES


REFERENCES


REFERENCES


REFERENCES


[DXL+10] Juan Du, Lili Xi, Beilei Lei, Jing Lu, Jiazhong Li, Huanxiang Liu, and Xiaojun Yao. Structure-based quantitative


Eller:2015:CAE


Ehara:2013:CII


Edel:2016:IFP


Erba:2013:ADS


Ehara:2016:PCS


Elenewski:2013:CPC

Justin E. Elenewski and John C. Hackett. Cytochrome P450 compound I in the plane wave pseudopotential framework: GGA electronic and geometric structure of thiolate-ligated

**El-Hamdi:2016:CAB**


**Eisenberg:2013:RTG**


**Eilmes:2015:SIT**


**Ehlert:2017:QBS**


**Ekesan:2014:TPE**


REFERENCES


[Hage:2015:CJL]


[Ellingson:2013:SNU]


[Eriksen:2012:IES]


[Ellis:2017:CDC]


[Eskandari:2014:HHI]


REFERENCES


[Anna Maria Ferrari, Bartolomeo Civalleri, and Roberto Dovesi. Ab initio periodic study of the conformational behavior of glycine helical homopeptides. *Journal of Computational
REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


Franchini:2013:BFC


Fraenkel:2015:ISL


Fraenkel:2016:ECI


Fuhrmann:2010:NLG


Fernandes:2015:QSL


Farahani:2014:RTS

REFERENCES


References

Fertitta:2014:AMA


Fernandez:2014:COA


Feng:2013:MGM


Fan:2015:DDS


Faraggi:2012:SXI


Glushkov:2012:OCM

V. N. Glushkov and X. Assfeld. On orthogonality constrained multiple core-hole states and optimized effective potential


Gavrish:2012:AER


Gumerov:2012:HAF


Gutsev:2016:SPI


Ganesan:2011:SDE


Gross:2017:MAI

Grebner:2011:ETS


Ghillemijn:2011:SCH


Grebner:2014:SNU


Gupta:2011:NDI


Gramatica:2014:SNU


[Gao:2017:IFP]

[Grimme:2011:EDF]


[Goldstein:2011:NHA]

[Ghasemi:2017:RDS]
Galvez:2010:TST


Gotze:2012:BHN


Georgieva:2010:QCM


Gross:2016:LED


Gross:2016:SNU


Gao:2012:AFE

REFERENCES


REFERENCES

Galstyan:2015:CPK


Gunera:2015:FBS


Gramatica:2013:LER


Glukhova:2014:MFB


Ghosh:2013:EFP

Gagnon:2016:FCD


Gan:2016:SIR


Gillet:2017:TER


Glendening:2013:ENN


Glendening:2013:SNU


Gao:2017:TSC


REFERENCES

1162, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Gonzalez-Navarrete:2012:EFD


Gonzalez-Navarrete:2010:DFT


Garate:2013:FED


Gonnet:2012:PVL


Granucci:2011:GCI


Gruber:2011:SBL

[GP11b] Christian C. Gruber and Jürgen Pleiss. Systematic benchmarking of large molecular dynamics simulations employing GROMACS on massive multiprocessing facilities. *Journal of
REFERENCES


**Gereben:2012:RCC**


**Gresh:2016:CZM**


**Grebner:2013:PGT**


**Gregori-Puigjané:2011:IMC**


**Gregori-Puigjané:2012:LER**

Elisabet Gregori-Puigjané, Rut Garriga-Sust, and Jordi Mestres. Letters to the editor: Response to the comment by Wolf Ihlenfeldt on the paper “Indexing molecules with chemical graph identifiers”. *Journal of Computational Chemistry*,
REFERENCES

Gusarov:2012:ETS

Ghara:2016:SSN

Geppert:2010:PPD

Genheden:2010:HOS

Grudinin:2010:PMM

Genheden:2011:CDI
Samuel Genheden and Ulf Ryde. A comparison of different initialization protocols to obtain statistically independent molecular dynamics simulations. *Journal of Computational Chem-
Grajciar:2015:LMI


Garcia-Risueno:2014:SPP


Gonzalez:2012:SRI


Giri:2010:BAS


Garcia-Risueno:2011:EEC

Grigoryan:2013:AFE


Guo:2011:PPF


Guo:2012:RRP

Jianxiu Guo, Nini Rao, Guangxiong Liu, Yong Yang, and Gang Wang. Retracted: Predicting protein folding rates using the concept of Chou’s pseudo amino acid composition. *Journal of Computational Chemistry*, 33(32):2614, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [GRL+11]. From the publisher: “The retraction has been agreed due to significant overlap with respect to another article, ‘Predicting Protein Folding Rate from Amino Acid Sequence,’ published in Progress in Biochemistry and Biophysics (2010, 37, 1331) and authored by a subset of the present authors.”.

Geppert:2012:VSC


Genheden:2015:BAA

Samuel Genheden, Ulf Ryde, and Pär Söderhjelm. Binding affinities by alchemical perturbation using QM/ MM with a


[GS16] Raimondas Galvelis and Yuji Sugita. The following articles were published in past issues of the *Journal of Computational Chemistry*: Replica state exchange metadynamics for improving the convergence of free energy estimates. *Journal of Computational Chemistry*, 37(6), March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Dimitrios N. Garbounis, Athanassios C. Tsipis, and Constantinos A. Tsipis. Structural, electronic, bonding, magnetic, and optical properties of bimetallic [Ru$_n$Au$_m$]$^{0/+}$ ($n + m \leq 3$
REFERENCES

Ghysels:2010:CSV

Ganesan:2011:IIP

Gutsev:2012:SPA

Gutsev:2011:DFS

Gan:2017:CCB
References


REFERENCES

953, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grinter:2014:BSA


Gan:2010:NFH


Gao:2012:MRN


Grosdidier:2011:FDU


Guo:2012:ICS


REFERENCES


REFERENCES


[HFSO12] Franziska Hess, Attila Farkas, Ari P. Seitsonen, and Herbert Over. “first-principles” kinetic Monte Carlo simulations re-


REFERENCES

Herrmann:2016:QCS

Hischenhuber:2013:CDG

Hischenhuber:2013:SNU

Huang:2017:EEB

Hill:2013:ABS


REFERENCES


[HL14] Bingjie Hu and Markus A. Lill. Software news and updates: WATsite: Hydration site prediction program with PyMOL.


Herbers:2013:RGC


Harger:2017:TOA


Huang:2015:ESM


Huang:2013:CAA


Hills:2016:MPS


Hongo:2010:RNG

Kenta Hongo, Ryo Maezono, and Kenichi Miura. Random number generators tested on quantum Monte Carlo simu-


REFERENCES

Heringer:2012:EAE


Hofener:2014:CCF


Harabuchi:2016:NST


Haque:2010:PAP


Henriksson:2010:PDT


He:2013:MPB


REFERENCES

Harano:2013:MAA


Husseini:2017:CIS


Huang:2017:EBE


Huwald:2016:CMD


Homann:2014:GOB


Hoffmann:2015:ECG

Alexander Hoffmann, Martin Rohrmüller, Anton Jesser, Ines dos Santos Vieira, Wolf Gero Schmidt, and Sonja Herres-

**Hahnke:2010:PAS**


**Huang:2011:CSR**


**Hernandez-Rodriguez:2013:EDD**


**Hahnke:2011:PASb**


**Helmich:2012:SRM**

Benjamin Helmich and Marek Sierka. Similarity recognition of molecular structures by optimal atomic matching and rotational superposition. *Journal of Computational Chemistry*,


REFERENCES


Zhaowei Huang, Hui Sun, Houyu Zhang, Yue Wang, and Fei Li. \(\pi-\pi\) interaction of quinacridone derivatives. *Journal of
Harada:2015:ECS


Harada:2017:CFP


Huang:2016:FSL

Bolong Huang. 4f fine-structure levels as the dominant error in the electronic structures of binary lanthanide oxides. *Journal of Computational Chemistry*, 37(9):825–835, April 5, 2016. CODEN JCCCHD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huggins:2012:BTA


Huggins:2014:CDM

REFERENCES


Hu:2016:QST


Huang:2010:IPE


Han:2011:END


Hoque:2016:SNU


Hori:2011:FEP

REFERENCES


REFERENCES


Atsushi Ishikawa and Hiroshi Nakatsuji. XPS of oxygen atoms on Ag(111) and Ag(110) surfaces: Accurate study with SAC/SAC-CI combined with dipped adcluster model. *Journal of Computational Chemistry*, 34(21):1828–1834, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Ishida:2010:BMH


Ishida:2012:FTG


Ikebe:2014:ALS


Imamura:2013:KED


Inui:2013:FFM


Illingworth:2010:CBS

REFERENCES


Jia:2017:EMI


Janesko:2016:TAE


Jacob:2011:DAP


Jacob:2011:PSF


Jaramillo-Botero:2011:LSL


Jahangiri:2014:PDF


Jaillet:2011:RTC


Jiang:2010:INA


Jorge:2017:PHSa


Jenkins:2013:SNU


Jimenez-Halla:2009:TAT


[JHMB+09]
Jimenez-Halla:2011:ETA


Jakobtorweihen:2013:CCM


Jiao:2016:CCS


Jin:2013:CPR


Joy:2016:CXZ

REFERENCES

Jeong:2014:SNU


Jankowska:2016:SOZ


Jia:2017:SNU


Jiang:2014:SCH


Jia:2010:CSM


369, March 5, 2017. CODEN JCCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


**Jin:2016:SCF**


**Jorgensen:2012:LEC**


**Jones:2016:MHD**


**Jensen:2015:ETS**


**Jono:2010:MIQ**

Ji:2015:IBL


Jin:2016:HAT


Jungsuttiwong:2012:ECS


Jafari:2017:RER

References

Johnston:2017:SDA


Jia:2014:AAP


Kunz:2012:SNU


Kantardjiev:2015:SNU


Koley:2012:CIC


[KB11c] Gerhard König and Stefan Boresch. Non-Boltzmann sampling and Bennett’s acceptance ratio method: How to profit from bending the rules. *Journal of Computational Chemistry*, 32
REFERENCES


REFERENCES


[KCPMG12] Hannes Kopitz, Daniel A. Cashman, Stefania Pfeiffer-Marek, and Holger Gohlke. Influence of the solvent representation...

Kalita:2010:ACO


Kessler:2013:PVS


Kumar:2017:CBD


Konc:2012:SNU


Kingsley:2016:RPP


Kaukonen:2012:LJP


Kramer:2012:AME


Kaupp:2016:ETP


Kearns:2017:CCF


Ko:2010:CIC

Kessler:2012:BEF


Kaliman:2017:SNU


Krause:2017:SNU


Kornobis:2013:ESS


Katouda:2011:TLH

REFERENCES


Michio Katouda, Akira Naruse, Yukihiko Hirano, and Takahito Nakajima. Massively parallel algorithm and implementation of RI-MP2 energy calculation for peta-scale many-core supercomputers. *Journal of Computational Chemistry*,
REFERENCES


Kjaer:2012:NMR


Karamanis:2014:SNO


Koput:2015:IGS


Koput:2015:ISC


Koput:2016:IPE

Koput:2017:IPEa


Koput:2017:IPEb


Kosenko:2016:SNU


Kowal:2011:IMG


Kim:2012:SHM


Kumar:2010:IEC


Goran Kovacevic and Aleksandar Sabljic. Theoretical study on the mechanism and kinetics of addition of hydroxyl radicals...


REFERENCES


Kokubo:2013:TDR


Klenin:2011:DMS


Kanematsu:2016:IUE


Kashmirian:2012:MDE


Kadam:2012:NAM


REFERENCES


Kumar:2015:SNU


Kirilchuk:2015:MPF


Kajiwara:2017:ITM


Koukaras:2012:SSE


Keceli:2016:SIP

REFERENCES


[Liu:2010:FDO] Pu Liu, Dimitris K. Agrafiotsis, and Douglas L. Theobald. Fast determination of the optimal rotational matrix for macro-

**Liu:2011:RCR**


**Lv:2016:CEH**


**Licari:2015:SNU**


**Laflamme:2012:SIS**


**Lucas:2012:MDS**

REFERENCES


Li:2010:NBO


Li:2015:VWE


Li:2010:TSH


Lorenz:2014:BDG


Liu:2016:DTI

REFERENCES

Lee:2013:NBO

Laury:2012:VFS

Lu:2010:FPS

Lesch:2017:SNU

Liu:2015:APE

Lyons:2014:PBC
[LDH$^+$14] James Lyons, Abdollah Dehzangi, Rhys Heffernan, Alok Sharma, Kuldip Paliwal, Abdul Sattar, Yaoqi Zhou, and Yue-

[LDJ+10] Qing-Zhong Li, Xu Dong, Bo Jing, Wen-Zuo Li, Jian-Bo Cheng, Bao-An Gong, and Zhi-Wu Yu. A new unconventional halogen bond $\text{C} \cdots \text{H} - \text{M}$ between HCCX (X = Cl and Br) and HMH (M = Be and Mg): an ab initio study. *Journal of Computational Chemistry*, 31(8):1662–1669, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES

2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Lin:2011:RPS

Li:2014:PDD

Liu:2012:SSH

Lee:2010:AUS

Lonsdale:2011:CSW

Le:2017:IDL
Nguyen-Quoc-Khanh Le, Quang-Thai Ho, and Yu-Yen Ou. Incorporating deep learning with convolutional neural networks and position specific scoring matrices for identifying


REFERENCES


REFERENCES


Li:2010:MLS


Liu:2010:TDT


Li:2011:TIG


Lee:2013:IMD


Liu:2013:EFA


Lai:2015:ICD


REFERENCES


[LLZA12] Chuan Li, Lin Li, Jie Zhang, and Emil Alexov. Software news and updates: Highly efficient and exact method for parallelization of grid-based algorithms and its implementation in


[LPE+10] Len Herald V. Lim, Andreas B. Pribil, Andreas E. Ellmerer, Bernhard R. Randolf, and Bernd M. Rode. Temperature dependence of structure and dynamics of the hydrated Ca$^{2+}$ ion according to ab initio quantum mechanical charge field


REFERENCES


Launay:2011:LDS


Liu:2011:EGS


Lei:2010:NIM


Liu:2011:ATD


Liao:2013:CQO


Liu:2014:OAC

Long:2011:CSU


Liu:2011:IMO


Lamiable:2016:CAH


Lu:2011:CSS


Luchow:2014:MPC


Ruifeng Lu, Yunhui Wang, and Kaiming Deng. Quantum wave packet and quasiclassical trajectory studies of the reaction H(^2S) + CH(\text{X}^2\text{II}) : v = 0, j = 1 \rightarrow C(^1\text{D}) + H2 (\text{X}^1\Sigma^+ g+) : Coriolis coupling effects and stereodynamics. *Journal of Computational Chemistry*, 34(20):1735–1742, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Xiao-Na Li, Zhi-Jian Wu, Xi-Yan Li, Hong-Jie Zhang, and Xiao-Juan Liu. Theoretical study on phosphorescence ef-


REFERENCES


[LYC+13] Yongqing Li, Jiuchuang Yuan, Maodu Chen, Fengcai Ma, and Mengtao Sun. Accurate double many-body expansion potential energy surface by extrapolation to the complete basis

**Li:2016:NSB**


**Liu:2011:TDS**


**Leis:2011:EIR**


**Lettieri:2012:AMM**


**Li:2014:MSP**

REFERENCES


[Li:2011:TDS] Qing-Zhong Li, Jun-Ling Zhao, Bo Jing, Ran Li, Wen-Zuo Li, and Jian-Bo Cheng. The structure, properties, and nature of HArF–HOX (X = F, Cl, Br) complex: an ab initio study.

**Li:2010:TDS**


**Liu:2013:FNM**


**Li:2015:CQM**


**Li:2015:CYX**

Wei Li, Yanli Zeng, Xiaoyan Li, Zheng Sun, and Lingpeng Meng. The competition of Y·O and X·N halogen bonds to enhance the group V σ-hole interaction in the NCY·o PH₃·NCX and O·PH₃·NCX·NCY (X, Y F, Cl, and Br) complexes. *Journal of Computational Chemistry*, 36(18):1349–1358, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

**Liu:2016:MIM**

Jiahui Liu, Yiyi Zheng, Ying Liu, Haiyan Yuan, and Jingping Zhang. Mechanistic insight on (E)-methyl 3-(2-aminophenyl)acrylate cyclization reaction by multicatalysis of


Martinez-Araya:2016:GOF


Mezey:2017:ASP


Michaud-Agrawal:2011:MTA


Matanovic:2014:ADF


Manz:2013:LEC


Mehdi:2010:ESR

[MAPB10] Ahmed Mehdi, Legesse Adane, Dhilon S. Patel, and Prasad V. Bharatam. Electronic structure and reactivity of guanylth-

**Matta:2010:HDM**


**Matta:2014:MBB**


**Maurice:2014:STF**


**Mogo:2014:SNU**


**Mogo:2016:SNU**

<table>
<thead>
<tr>
<th>Reference</th>
<th>Authors</th>
<th>Title</th>
<th>Journal</th>
<th>Volume</th>
<th>Pages</th>
<th>Date</th>
<th>CODEN</th>
<th>ISSN</th>
</tr>
</thead>
<tbody>
<tr>
<td>MBA11</td>
<td>Alessandra Manzin, Oriano Bottauscio, and Domenico Patrizio Ansalone</td>
<td>Application of the thin-shell formulation to the numerical modeling of Stern layer in biomolecular electrostatics</td>
<td>Journal of Computational Chemistry</td>
<td>32(14)</td>
<td>3105–3113</td>
<td>November 15, 2011</td>
<td>JCCHDD</td>
<td>0192-8651 (print), 1096-987X (electronic)</td>
</tr>
<tr>
<td>MBC11</td>
<td>Michel Masella, Daniel Borgis, and Philippe Cuniasse</td>
<td>Combining a polarizable force-field and a coarse-grained polarizable solvent model. II. Accounting for hydrophobic effects</td>
<td>Journal of Computational Chemistry</td>
<td>32(12)</td>
<td>2664–2678</td>
<td>September 2011</td>
<td>JCCHDD</td>
<td>0192-8651 (print), 1096-987X (electronic)</td>
</tr>
<tr>
<td>MBFG15</td>
<td>Krishnakanta Mondal, Arup Banerjee, Alessandro Fortunelli, and Tapan K. Ghanty</td>
<td>Does enhanced oxygen activation always facilitate CO oxidation on gold clusters?</td>
<td>Journal</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**REFERENCES**


REFERENCES

2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


REFERENCES


Mollenhauer:2011:AQC


Morao:2017:RAA


Micera:2011:SOC


Mollenhauer:2014:BPT


Marmitt:2015:DSI


Tetsuya Morishita, Satoru G. Itoh, Hisashi Okumura, and Masuhiro Mikami. On-the-fly reconstruction of free-energy

**Muhammad:2015:HDH**


**Mitin:2013:PFM**


**Maingi:2012:DBT**


**Martin:2014:CAN**


**Mones:2015:ABF**

Letif Mones, Andrew Jones, Andreas W. Götz, Teodoro Laino, Ross C. Walker, Ben Leimkuhler, Gábor Csányi, and Noam Bernstein. The adaptive buffered force QM/MM

Marx:2014:CLH


Marx:2014:MMS


Mitoraj:2015:NWA


Mach:2011:GML


Mach:2013:AMC

Malyszek:2013:AIP


Moore:2013:HQP


Makowski:2010:DEC


Merlot:2013:AEE


Middendorf:2015:SSB


Miyashita:2017:FFC

Matsui:2013:CSC


Marais:2012:ECM


Mirzoev:2014:SIS


Mohammed:2013:FOF


Mok:2011:FCS

Makarewicz:2016:NIF


Ma:2012:TIR


Mo:2013:DSE


Mei:2012:EPC


Masetti:2017:DMM


Katsumi Murata, Naoya Nagata, Isao Nakanishi, and Kazuo Kitaura. Ligand shape emerges in solvent dipole ordering


Mitra:2011:UCP


Marques:2013:DIG


Myers:2017:PLP


Marques:2010:GCL


Marques:2012:UBB


Mukherjee:2011:FEG

Goutam Mukherjee, Niladri Patra, Poranjyoti Barua, and B. Jayaram. A fast empirical GAFF compatible partial atomic charge assignment scheme for modeling interactions of small

**Minovski:2013:CBM**


**Mahanta:2011:ISP**


**Miriayala:2017:DNC**


**Mandado:2014:AER**


**Meisner:2011:KIE**

REFERENCES


REFERENCES

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muller:2015:CSN


Mignon:2016:CTS


Mahajan:2017:JBP


Mishra:2012:CPM


Matta:2016:BMR

REFERENCES

Marsili:2010:OMD


Malolepsza:2010:SAC


Malolepsza:2012:ESA


Maciejczyk:2010:CGM


Mayne:2013:RPS

Martinez:2016:TER


Meier:2012:IGB


Maeda:2014:ETS


Meier:2012:EVF


Mohammadiarani:2017:IMP


Mohan:2010:CAN

Neetha Mohan, Kunduchi P. Vijayalakshmi, Nobuaki Koga, and Cherumuttathu H. Suresh. Comparison of aromatic

Miao:2011:DFT


Matsuzaki:2017:CPD


Matsuzaki:2017:OCS


Maruyama:2014:MPI


Mamonov:2011:RSA

Nemoto:2015:ISN


Neogi:2012:SSW


Neogi:2013:SSA


Neogi:2014:SSA


Nemeth:2010:CIC


Noel:2010:USI

Yves Noel, Philippe D’arco, Raffaella Demichelis, Claudio M. Zicovich-Wilson, and Roberto Dovesi. On the use of symmetry in the ab initio quantum mechanical simulation of nanotubes.


Nozaki:2016:TSL


Nickerson:2013:CCW


Noy:2010:FPP


Najeh:2010:ETS


Nowosielski:2013:MTC


[NLP+16] Christophe Narth, Louis Lagardère, Étienne Polack, Nohad Gresh, Qiantao Wang, David R. Bell, Joshua A. Rackers,


[NMLD13] Maggie Ng, Daniel K. W. Mok, Edmond P. F. Lee, and John M. Dyke. Rate coefficients of the $\text{CF}_3\text{CHFCF}_3 + \text{H} \rightarrow \text{CF}_3\text{CFCF}_3 + \text{H}_2$ reaction at different temperatures calculated by transition state theory with ab initio and DFT reaction paths. *Journal of Computational Chemistry*, 34(7):545–557, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Nishizawa:2016:RQM


Norby:2016:MME


Ng:2017:RFT


Nunes:2013:NAP


Nagai:2016:UMS

REFERENCES


gust 5, 2015. CODEN JCCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


[OAN15a] Masaki Okoshi, Teruo Atsumi, and Hiromi Nakai. Revisiting the extrapolation of correlation energies to complete basis
REFERENCES


Ootani:2015:TIE


Oehme:2012:EAC


Ozkanlar:2014:SNU


Olson:2011:CBS


Ortega-Carrasco:2014:APL


Osman:2016:RPS


Okoshi:2014:ASC


Ortega:2016:CEN


Ozawa:2011:ICH


Otsuka:2015:AAB


Otero:2015:HBI


Opron:2016:FRI


Okamoto:2011:MIA


Ostermeir:2014:HRE


Ouk:2012:TST

REFERENCES


Pietropaolo:2011:CBM


Perilla:2011:CET


Porsev:2016:TDS


Palma:2012:CBA


Patra:2011:ANN


Pelloni:2014:CCS

Stefano Pelloni and Inmaculada García Cuesta. CCSD–CTOCD static dipole shielding polarizability for quantifica-

**Pritchard:2016:HVE**


**Pelloni:2011:RCM**


**Plumley:2011:CBF**


**Plazinski:2012:DCI**


**Pinjari:2016:CSR**


Pan:2012:CSH


Pacios:2012:CSL


Paschoal:2016:PPN


Pantazes:2015:SNU


Pan:2015:CCS

Pirojsirikul:2017:CQM


Panteva:2015:CST


Pesonen:2010:PCI


Poolmee:2010:IES


Panosetti:2012:AMC


Proppe:2015:CTM

[PH15] Jonny Proppe and Carmen Herrmann. Communication through molecular bridges: Different bridge orbital trends re-

Passler:2017:CLM

PH17


Pang:2013:SEM

PHC13


Pape:2013:DDM

PHDH13


Pool:2012:SNU

PHH+12


Pedersen:2014:BSE

PHK14

REFERENCES


[Papp:2017:TIN] Tamara Papp, László Kollár, and Tamás Kégl. Theoretical insights into the nature of Pt–Sn bond: Reevaluating the bonding/back-bonding properties of trichlorostannate with comparison to the cyano ligand. *Journal of Computational Chem-
REFERENCES


Pezeshki:2014:MDS

Plazinski:2011:MBC

Plewczynski:2011:CWT

Plazinski:2016:RGF

Presti:2016:MEF


REFERENCES

CODEN JCCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


<table>
<thead>
<tr>
<th>Reference</th>
<th>Title</th>
<th>Authors</th>
<th>Journal</th>
<th>Volume</th>
<th>Issue</th>
<th>Pages</th>
<th>Year</th>
<th>CODEN</th>
<th>ISSN</th>
</tr>
</thead>
</table>


Purushotham:2012:CIC


Popo:2013:SNU


Plessow:2012:SNU


Pang:2010:SOS


Pyykko:2013:REB

Petukh:2015:SIS


Pinsky:2013:CSA


Peng:2016:FES


Porta:2015:HHB


Quapp:2010:CNE


Quapp:2011:RCS

REFERENCES


Randic:2013:VES


Rao:2011:PIS


Rathore:2011:MMS


Raskovalov:2017:SNU


Rayne:2013:LEC


Ricci:2012:DFT

REFERENCES

Rai:2013:FAG


Rice:2013:EED


Robinson:2011:WOP


Ren:2013:UEE

[RCM+13a] Yanliang Ren, Bo Chi, Osama Melhem, Ke Wei, Lingling Feng, Yongjian Li, Xinya Han, Ding Li, Ying Zhang, Jian Wan, Xin Xu, and Minghui Yang. Understanding the electronic energy transfer pathways in the trimeric and hexameric aggregation state of cyanobacteria phycocyanin within the framework of fürster theory. *Journal of Computational Chemistry*, 34(12):1005–1012, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roy:2013:SNU


anions: Charge and energy analysis of [Sn$_2$ E$_2^{15}$ (ZnPh)$_2$]$^{3-}$ (E$^{15}$ = Sb, Bi) and [Sn$_2$ Sb$_5$ (ZnPh)$_2$]$_3^{3-}$. *Journal of Computational Chemistry*, 35(14):1045–1057, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Amir Abbas Rafati, Sayed Majid Hashemianzadeh, Zabiololah Boli Bolbol Nojini, and Negin Naghshineh. Canonical Monte Carlo simulation of adsorption of O2 and N2 mixture on single walled carbon nanotube at different temperatures and pressures. *Journal of Computational Chemistry*, 31(7):1443–1449,
Rohrmuller:2013:BMO


Racine:2016:RWF


Rohrmuller:2015:CTT


Rui:2010:POP


Rick:2016:PCT


[Rusak\textsuperscript{o}v\textsuperscript{i}2015:FCR] Yury Yu. Rusakov and Leonid B. Krivdin. Four-component relativistic DFT calculations of $^{77}$Se NMR chemical shifts: a

**Rossini:2016:EPS**


**Rossini:2016:PSP**


**Romero:2014:PDU**


**Roston:2014:SRM**


**Roy:2011:QMR**

REFERENCES


REFERENCES

Rehman:2016:SS


Ramirez-Manzanares:2015:HAM


Rogers:2017:PDM


Randic:2013:CVMa


Ramsey:2016:SNU


Randic:2013:CVMb

Reif:2014:MDS


Reif:2014:NCC


Robinson:2013:SMB


Rodriguez:2013:EMC


Randić:2015:PAE


Randić:2010:NGD

References}


Karunakaran Remya and Cherumuttatu H. Suresh. Cooperativity and cluster growth patterns in acetonitrile: a DFT


REFERENCES


REFERENCES


Reif:2016:RAC


Rao:2013:NPL


Sattelle:2010:LMW


Swetnam:2011:IWL


Schumann:2013:SES


Spivak:2014:ICM

[SACdG\textsuperscript{14}] Mariano Spivak, Celestino Angeli, Carmen J. Calzado, and Coen de Graaf. Improving the calculation of magnetic cou-

**Scemama:2016:QMC**


**Sanchez:2017:RTC**


**Szklarczyk:2015:PCG**


**Sax:2012:LMO**


**Salehzadeh:2010:TSS**


**Silva:2011:HFO**

Alexander M. Silva and Itamar Borges Jr. How to find an optimum cluster size through topological site properties: MoS$_x$

**Stepanek:2013:CMC**


**Soydas:2014:AOO**


**Stepanek:2015:OIS**


**Sedeh:2010:SIM**


**Simpson:2011:EIC**


REFERENCES

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2012:IPM


Sibaev:2015:SNU


Scerri:2007:PTS


Schwarz:2010:BRB


Schwabe:2012:AFT

References

Schmidling:2013:NSB


Sanchez:2015:NQM


Song:2017:SDI


Scemama:2013:QMC


Song:2013:EAC


Selvam:2011:MZI


REFERENCES

Suarez:2013:SNU


Shen:2017:ECC


Shirazi:2014:AKM


Seal:2010:CRG


Shaghaghi:2016:SGA


Solomentsev:2012:EEE

Gleb Y. Solomentsev, Niall J. English, and Damian A. Mooney. Effects of external electromagnetic fields on the conformational sampling of a short alanine peptide. *Journal of


REFERENCES


Elsa Sanchez-Garcia, Markus Doerr, and Walter Thiel. QM/MM study of the absorption spectra of DsRed.M1 chro-
REFERENCES


REFERENCES


REFERENCES


[SHMO11] Yoshitake Sakae, Tomoyuki Hiroyasu, Mitsunori Miki, and Yuko Okamoto. Protein structure predictions by parallel sim-


[SJ16] Pin-Chih Su and Michael E. Johnson. Evaluating thermodynamic integration performance of the new Amber molecular dynamics package and assess potential halogen bonds of enoyl-ACP reductase (FabI) benzimidazole inhibitors. *Journal of
REFERENCES


Song:2015:ODO


Szarek:2011:MED


Sharma:2012:CPK


Stachowicz:2013:BDM


Sakalli:2015:PKP


Schultz:2015:SNU

REFERENCES


molecular structures of X-, α-, and β-types of lithium phthalo-
3062–3067, November 15, 2011. CODEN JCCHDD. ISSN
0192-8651 (print), 1096-987X (electronic).

Safi:2010:RDE

[SL10] Maria Safi and Ryan H. Lilien. Restricted dead-end elimin-
ation: Protein redesign with a bounded number of residue
1215, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651
(print), 1096-987X (electronic).

Surakhot:2017:TRR

[SLC+17] Yaowarat Surakhot, Viktor Laszlo, Chirawat Chitpakdee,
Vinich Promarak, Taweesak Sudyoadsuk, Nawee Kungwan,
Tim Kowalczyk, Stephan Irle, and Siriporn Jungsuttiwong.
Theoretical rationalization for reduced charge recombination
in bulky carbazole-based sensitizers in solar cells. *Journal
CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (elec-
tronic).

Stenrup:2015:CNG

Constrained numerical gradients and composite gradients:
Practical tools for geometry optimization and potential en-
ergy surface navigation. *Journal of Computational Chemistry*,
36(22):1698–1708, August 15, 2015. CODEN JCCHDD. ISSN
0192-8651 (print), 1096-987X (electronic).

Song:2009:ETS

[SLHW09] Xinli Song, Jicun Li, Hua Hou, and Baoshan Wang. Extensive
theoretical studies of a new energetic material: Tetrazino-
tetrazine-tetraoxide (TTTO). *Journal of Computational
Chemistry*, 30(12):1816–1820, September 2009. CODEN JC-
CHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See
[JW12].

Sladek:2012:ICS

[SLIB12] Vladimír Sládek, Vladimír Lukeš, Michal Ilčín, and Stanislav
Biskupič. Ab initio calculation of structure and transport
properties of He...X (X = Zn, Cd, Hg) van der Waals com-
plexes. *Journal of Computational Chemistry*, 33(7):767–778,
March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print),
1096-987X (electronic).

[SLLL13] Jen-Ping Su, Yung-Ting Lee, Shao-Yu Lu, and Jyh Shing
Lin. Chemical mechanism of surface-enhanced Raman scatter-
ing spectrum of pyridine adsorbed on Ag cluster: Ab ini-
tio molecular dynamics approach. *Journal of Computational
JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

[SLP+12] Volker Settels, Wenlan Liu, Jens Pflaum, Reinhold F. Fink,
and Bernd Engels. Comparison of the electronic structure of
different perylene-based dye-aggregates. *Journal of Compu-
JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

[Sala:2014:SET] Oliver Sala, Hans Peter Lüthi, and Antonio Togni. The sol-
vent effect on two competing reaction mechanisms involving
hypervalent iodine reagents ($\lambda^3$-iodanes): Facing the limit of
the stationary quantum chemical approach. *Journal of Compu-
CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (elec-
tronic).

[Sala:2015:DCR] Oliver Sala, Hans Peter Lüthi, Antonio Togni, Marcella Ian-
nuzzi, and Jürg Hutter. Dividing a complex reaction involv-
ing a hypervalent iodine reagent into three limiting mecha-
nisms by ab initio molecular dynamics. *Journal of Compu-
JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

[Shen:2015:ACG] Hujun Shen, Yan Li, Peijun Xu, Xiaofang Li, Huaying Chu,
Dinglin Zhang, and Guohui Li. An anisotropic coarse-grained
model based on Gay–Berne and electric multipole potentials
and its application to simulate a DMPC bilayer in an implicit
1103–1113, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651
(print), 1096-987X (electronic).


[SM16a] Sadegh Salehzadeh and Farahnaz Maleki. New equation for calculating total interaction energy in one noncyclic ABC triad and new insights into cooperativity of noncovalent

**Stachiewicz:2016:DDD**


**Szczepaniak:2017:ARB**


**Sheng:2011:CCU**


**Sumi:2015:ESF**


**Sumi:2015:SFE**


[SN16b] Junji Seino and Hiromi Nakai. Informatics-based energy fitting scheme for correlation energy at complete basis set
REFERENCES


REFERENCES


Springborg:2010:BRB  

Sousa:2013:CAP  

Saha:2012:CSS  

Strohecker:2010:QCI  

Szalay:2011:FCD  
Sakkal:2017:PCB


Savarese:2017:CPT


Shyichuk:2015:SDC


Sengupta:2016:BBA


Smith:2014:SES

REFERENCES


Julia Setzler, Carolin Seith, Martin Brieg, and Wolfgang Wendel. SLIM: an improved generalized Born implicit membrane...
REFERENCES


Pin-Chih Su, Cheng-Chieh Tsai, Shahila Mehboob, Kirk E. Hevener, and Michael E. Johnson. Comparison of radii sets,

**Sumiya:2017:FRC**


**Sun:2010:TKS**


**Sure:2015:SSR**


**Su:2010:CSP**


**Sun:2015:LEG**


Weiyu Song, Jing Wang, Jian Meng, and Zhijian Wu. Half metallic properties of LaSrVMoO$_6$. *Journal of Computational
Shi:2011:MEH


Shyu:2011:AES


Spassov:2016:PDC


Su:2016:TDT


Sharabi:2011:OEF


Sindhikara:2012:PAP

REFERENCES

1536–1543, July 5, 2012. CODEN JCCCHD. ISSN 0192-8651 (print), 1096-987X (electronic).

Solovyov:2012:MEU


Sun:2017:AVW


Shim:2013:AXA


Schupbach:2010:FTC


Su:2013:ADX

REFERENCES


Takahashi:2014:DRF


Tan:2012:CSP


Tantardini:2016:SFP


Thomas:2013:PGF


Torres:2014:TSR

Ana E. Torres, Guadalupe Castro, Ricardo Pablo-Pedro, and Fernando Colmenares. A two-step reaction scheme leading to singlet carbene species that can be detected under matrix conditions for the reaction of Zr(3 F) with either CH3F or CH3CN. *Journal of Computational Chemistry*, 35(11):883–890, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tu:2013:PFE

Bin Tu, Minxin Chen, Yan Xie, Linbo Zhang, Bob Eisenberg, and Benzhuo Lu. A parallel finite element simula-


[TF15] Russell Thackston and Ryan C. Fortenberry. The performance of low-cost commercial cloud computing as an alternative in computational chemistry. *Journal of Computational Chem-


[Teodoro:2013:ARA] Tiago Quevedo Teodoro and Roberto Luiz Andrade Haiduke. Accurate relativistic adapted Gaussian basis sets for francium through ununoctium without variational prolapse and to be used with both uniform sphere and Gaussian nucleus models.
REFERENCES


[TLdG+12] Zahra Tabookht, Xavier López, Coen de Graaf, Nathalie Guihéry, Nicolas Suaud, and Nadia Benamor. Rationalization of the behavior of $M_2\left(\text{CH}_3\text{CS}_2\right)_4\text{I}$ ($M = \text{Ni, Pt}$) chains at room temperature from periodic density functional theory

[Tang:2012:CFF]


[Tahat:2016:MEV]


[Tognetti:2015:QEN]


[Takano:2010:ESH]


[Tai:2012:EST]


Thenraj:2015:CER


Tsipis:2015:EBO

Athanassios C. Tsipis and Alexandros V. Stalikas. Electronic, bonding, and optical properties of 1 d [CuCN]_n (n = 1–10) chains, 24 d [Cu CN]_n (n = 2–10) nanorings, and 3 d [Cu_n (CN)_m]_n (n = 4, m = 2, 3; n = 10, m = 2) tubes studied by DFT /TD–DFT methods. *Journal of Computational Chemistry*, 36(17):1334–1347, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Thellamurege:2013:SNU


Tsipis:2014:DAS


Tsipis:2017:EPR

Tang:2010:MKI


Tsuneda:2016:RBO


Tsuneda:2017:LLE


Torres:2016:SAA


Tang:2012:TMG


Toropov:2010:SBO

REFERENCES


REFERENCES


(26):2341–2348, October 5, 2016. CODEN JCCCHDD. ISSN
0192-8651 (print), 1096-987X (electronic).

\textbf{Udagawa:2011:IMD}

[U11] Taro Udagawa and Shogo Sakai. Ab initio molecular dy-
namics of protonated water clusters by integrated multicenter molecular-orbital method. \textit{Journal of Computational Chem-

\textbf{Udagawa:2014:WND}

[UT14] Taro Udagawa and Masanori Tachikawa. Why is N···Be distance of NH$_3$H$^+$···DBeH shorter than that of NH$_3$D$^+$···HBeH$^+$? Paradoxical geometrical isotope effects for partially isotope-substituted dihydrogen-bonded isotopomers. \textit{Journal of Com-
putational Chemistry}, 35(4):271–274, February 5, 2014. CO-
DEN JCCCHDD. ISSN 0192-8651 (print), 1096-987X (elec-
tronic).

\textbf{Udagawa:2015:HDI}

[UT15] Taro Udagawa and Masanori Tachikawa. H/D isotope ef-

\textbf{Uejima:2011:AQM}


\textbf{Ullmann:2012:SNU}

REFERENCES


Vogt:2014:WIS


Vener:2012:IHB


VonAppen:2010:DFS


Vela:2016:ZOH


Vogt-Geisse:2016:CPR


REFERENCES


[VSD10] Santhosh Kannan Venkatesan, Anil Kumar Shukla, and Vikash Kumar Dubey. Molecular docking studies of selected

**vanSeveren:2010:ATA**


**VanDornshuld:2014:CPE**


**Viegas:2014:CCR**


**Vanpoucke:2013:LER**


**Vega-Vega:2017:MMC**

REFERENCES

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


Vincent A. Voelz and Guangfeng Zhou. Bayesian inference of conformational state populations from computational mod-


Wan:2011:MDS

Wang:2013:HWM

Wise:2014:NFF

Wu:2010:QMS

Weill:2011:TCT


Wang:2011:ELP


Wessel:2010:FPS


Wu:2013:PFB


Wang:2012:DFT


Wu:2012:QCI


Wagener:2012:SNU


**Wilson:2012:PHE**


**Waller:2013:SNU**


**Wang:2016:RMR**


**Weinhold:2012:NBO**


**Weinhold:2012:SNU**


**Watanabe:2013:RDP**

[WES13] Hiroshi Watanabe, Marcus Elstner, and Thomas Steinbrecher. Rotamer decomposition and protein dynamics: Efficiently an-


REFERENCES


REFERENCES

Wolf:2016:ECG


Wu:2011:TMS


Will:2013:SNU


Weymuth:2012:SNU


Wang:2010:TDD


Benjamin Waldher, Jadwiga Kuta, Samuel Chen, Neil Henson, and Aurora E. Clark. ForceFit: a code to fit classical force


REFERENCES

Wallnoefer:2011:CSF


Wang:2012:HAR


Witzke:2017:APP


Wang:2010:EET


Wu:2012:LER


Wuttke:2017:VDI

[Axel Wuttke and Ricardo A. Mata. Visualizing dispersion interactions through the use of local orbital spaces. *Journal


REFERENCES


REFERENCES

Wang:2010:BCA

Wirz:2016:SFG
Lukas N. Wirz, Ralf Tonner, Andreas Hermann, Rebecca Sure, and Peter Schwerdtfeger. From small fullerenes to the graphene limit: a harmonic force-field method for fullerenes and a comparison to density functional calculations for Goldberg–Coxeter fullerenes up to C_{980}. *Journal of Computational Chemistry*, 37(1):10–17, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2010:CCN

Weinhold:2014:BTH

Wang:2015:BCD

Wenzel:2014:CCL
Jan Wenzel, Michael Wormit, and Andreas Dreuw. Calculating core-level excitations and X-ray absorption spectra


REFERENCES


[Wang:2017:ARS] Chao Wang, Yizhong Yuan, and Xiaohui Tian. Assessment of range-separated exchange functionals and nonempirical func-


REFERENCES


[XhD15] Jing Xu and Yi hong Ding. Pentaatomic planar tetracoordinate silicon with 14 valence electrons: a large-scale global search of SiX$_m$Y$^q_m$ ($n + m = 4$; $q = 0, \pm 1, -2$; X, Y = main group elements from H to Br). *Journal of Computational Chemistry*, 36(6):355–360, March 5, 2015. CODEN JCCCHD. ISSN 0192-8651 (print), 1096-987X (electronic).


REFERENCES


Yu:2011:ETS


Yamamoto:2013:TPM


Yildiz:2016:AEK


Yu:2010:TSN


Youn:2016:EEF


Yang:2017:ERV

Chong Yang and Andreas Dreuw. Evaluation of the restricted virtual space approximation in the algebraic-diagrammatic

[Yuan:2015:TPH]


[Yao:2010:SDS]


[Yang:2013:RWA]


[Yu:2016:PKP]


[Yesylevskyy:2012:SNU]

Yesylevskyy:2015:SNU

Yu:2011:AMA

Yang:2011:TSG

Yu:2013:SNU

Yu:2012:ECG
Yao:2013:MDS


Yeh:2011:DFT


Yu:2017:PDS


Yourdkhani:2017:RPN


Yakhanthip:2011:TIN


Yu:2017:PS
REFERENCES

Yamada:2013:VDE


Yan:2010:CSE


Yourdkhani:2015:IBT


Yamada:2011:TNA


Yuzlenko:2013:MPN


Yoshikawa:2015:LSS


Yamaguchi:2017:RRA


Ou:2010:PMS


Yamagishi:2014:NSA


Yonezawa:2016:MPP


Yu:2016:DAS

REFERENCES

2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).


[YR13] Rui Yang and Alistair P. Rendell. First principles study of gallium cleaning for hydrogen-contaminated α-Al2O3 (0001)

**Yu:2010:RPC**


**Yoshizawa:2013:NSC**


**Yosipof:2015:KNN**


**Yang:2012:GAN**


**Yousfi:2010:REM**


**Yang:2012:MZE**

[YSSB12] Hongfang Yang, Qisheng Song, Xinyu Song, and Yuxiang Bu. Multi-zinc-expanded graphene patches: Tetraradical versus

**[Yu:2012:IDC]**


**[Yu:2012:AIM]**


**[Yanez:2017:FF]**


**[Yanez:2017:FF]**


**[Yan:2012:ESL]**


**[Yang:2013:RNI]**


Sheng-Chun Yang, Yong-Lei Wang, Gui-Sheng Jiao, Hu-Jun Qian, and Zhong-Yuan Lu. Software news and updates: Ac-

Yang:2014:VSP


Yu:2012:TSE


Yan:2015:PPB


Yuan:2015:DHH


Yang:2016:EPC

REFERENCES


Bo Yang, Yanyan Zhu, Yan Wang, and Guangju Chen. Interaction identification of Zif268 and TATA$_{ZF}$ proteins with


REFERENCES


[ZCS+15] Shenggao Zhou, Li-Tien Cheng, Hui Sun, Jianwei Che, Joachim Dzubiella, Bo Li, and J. Andrew McCammon. LS-


REFERENCES

____

Zhang:2011:SSE


Zhang:2012:REFb


Zhang:2012:REFa


Zou:2011:SSP


Zimmerman:2013:ADC


Zimmerman:2015:SET


[ZLL+10] Laibin Zhang, Huifang Li, Jilai Li, Xiaohua Chen, and Yuxiang Bu. Absorption and fluorescence emission spectroscopic

**Zhu:2013:SNU**


**Zhang:2012:TSRb**

[ZLLL12] Hui Zhang, Yang Liu, Jing-Yao Liu, and Ze-Sheng Li. Theoretical study and rate constants calculation for the reactions \( X + \text{CF}_3\text{CH}_2\text{OCF}_3 \) (\( X = \text{F}, \text{Cl}, \text{Br} \)). *Journal of Computational Chemistry*, 33(6):685–690, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

**Zhang:2015:EMC**


**Zhang:2013:ICA**


**Zheng:2010:ITA**

Zheng:2013:WPP


Zhao:2016:LPT

Xue-Feng Zhao, Haixia Li, Cai-Xia Yuan, Yan-Qin Li, Yan-Bo Wu, and Zhi-Xiang Wang. Linear, planar, and tubular molecular structures constructed by double planar tetracoordinate carbon D$_{2h}$ C$_2$ (BeH)$_4$ species via hydrogen-bridged BeH$_2$Be bonds. *Journal of Computational Chemistry*, 37(2):261–269, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2014:ECM


Zhu:2010:PEF


Zoboki:2011:ELN


Zhang:2012:IRE

REFERENCES

43, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhong:2013:BST


Zarbeto:2014:LSF


Zarycz:2016:CSB


Zhu:2014:TPC


Zilberberg:2010:POD


Zapata-Rivera:2011:ESR

Jhon Zapata-Rivera, Rosa Caballol, and Carmen J. Calzado. Electronic structure and relative stability of 1:1 Cu-O₂

**Zapata-Rivera:2012:RML**


**Zgarbova:2015:TAD**


**Zare-shahabadi:2010:AAC**


**Zadeh:2011:NAD**


**Zoete:2016:ACD**

Zhao:2011:CDL


Zhan:2017:ASE


Zhao:2013:FPC


Zahariev:2014:FAM


Zhang:2012:DFT

REFERENCES


Zhou:2015:ABO


Zaccaria:2016:IST


Zhang:2013:MPI


Zhang:2011:ABD


Zhao:2010:PSM


Zadeh:2011:NAS

REFERENCES

February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2010:MDM


Zhao:2010:SSP


Zhou:2016:IBH


Zheng:2010:DFTb


Zheng:2010:DFTa

Zhang:2011:IIR


Zhao:2011:HMM


Zhang:2010:ESO


Zhao:2014:IDB


Zhao:2014:DSE


Zhang:2015:TCS

[ZYG+15]  Xu Zhang, Xiaodi Yang, Hua Geng, Guangjun Nan, Xingwen Sun, Jinyang Xi, and Xin Xu. Theoretical comparative studies on transport properties of pentacene, pentathienoacene, and

**Zhu:2012:PPT**


**Zhang:2012:TSRa**


**Zhao:2015:PRM**


**Zhu:2010:IAP**


**Zhao:2014:CBP**

Zhao:2016:CDO


Zhang:2010:III


Zhou:2012:CMF


Zeller:2014:ECR


Zhang:2010:TSRb


Zhang:2010:TSRa

[ZZL⁺10b] Hui Zhang, Gui-Ling Zhang, Jing-Yao Liu, Miao Sun, Bo Liu, and Ze-Sheng Li. Theoretical study and rate constants cal-

**Zeng:2012:AII**


**Zhang:2012:RMC**


**Zhu:2011:CSE**


**Zhang:2016:CQD**