Appendix E

Supplemental Data for Table 10-1. Selected 1,7-$C_2B_{10}H_{12}$ Derivatives

Compound[a]	Information[b]	References
Nontransition metal derivatives		
Parent	S	[20,27]
	C	[20]
	IR	[21,45]
	Photoemission spectra, MO binding energies, absorption on metal surfaces	[61]
	Molecular films, photoemission and inverse photoemission studies	[611]
	Dipole moment	[67,68]
	Dielectric data, relaxation dynamics, plastic crystals	[69]
	Ionic fragmentation following photon-induced B 1 s and C 1 s excitation vs. energetics of decomposition	[70]
	Filler in polydimethylsiloxane bimodal networks; segmental dynamics	[809]
	Photo-fragmentation, double cation formation photoelectron-photoion-photoion coincidence (PEPIPICO) spectroscopy; MS (time-of-flight mass analysis)	[866]
1,7-$C_2B_{10}H_{12}$ boronization of tokakamak walls (FF)		[821]
Alkyl derivatives		
1-Me	C	[80,81]
	IR	[22]
1-Me-7-Et	S	[84]
1-Me-7-Ph	S	[77]
1,7-(*n*-C_3H_7)$_2$	S	[78]
1-$CHMe_2$	S	

Compound	Information	References
1-C_3H_7-7-*i*-C_4H_9	S	[87]
1-*n*-C_4H_9	Heat of evaporation, vapor pressure	[88]
1-*i*-C_4H_9	Heat of evaporation, vapor pressure	[88]
1,7-(*n*/*i*-$C_4H_9)_2$	S	[87]
1-C_5H_{11}	Heat of evaporation, vapor pressure	[88]
1,7-$(C_5H_{11})_2$	S	[87]
1-C_6H_{13}	Heat of evaporation, vapor pressure	[88]
1,7-$(CR_2$-$C_5H_5)_2$ R$_2$=Me$_2$, $(CH_2)_5$	S, H, B	[89]
1,7-$(C_6H_{13})_2$	S	[87]
1,7-$(C_{10}H_{21})_2$	S	[87]
n-(*n*-C_4H_9) *n*=4, 5, 9	S (electrophilic alkylation)	[92]
9-*n*-C_3H_7	S	[96]
9-*n*-C_4H_9	S {Pd[$PPh_3]_4$ catalyzed}	[97]
	S (from RMgX)	[95,98]
9-C_6H_{13}	S	[96]
Haloalkyl derivatives		
1-CH_2CH=$CHCH_2$R R=*n*-C_6F_{13}, *i*-C_3F_7	S, H, B, C, F, IR, MS	[101]
1-CH_2Cl	Dipole moment	[344]
1,7-$(C_2H_4Cl)_2$	S	[102]
1-(*n*-C_3H_6-3′-Cl)	S	[102]
1-(*n*-C_8H_{16}-8′-Cl)	S	[102]
1-CH_2X-7-R R=H, Me; X=Cl, Br	S	[103]
	Dipole moment	[344]
1-$(CH_2)_3$X-B-Me$_8$ X=Cl, Br	S, H, B, C, MS	[105]
[Br$(CH_2)_3$]HC_2B_{10}Me$_8H_2$ (FF)	S, H, B, C, MS	[194]
[Br$(CH_2)_n]_2C_2B_{10}$Me$_8H_2$ *n*=3, 4 (FF)	S, H, B, C, MS	[194]
1,7-(*n*-C_4H_9-4′-Br)$_2$	S	[102]
1-C_2H_4Br	S	[102]
1,7-(C_2H_4-2′-Br)$_2$	S	[102]
1-(*n*-C_6H_{12}-6′-Br)	S	[102]
1,7-$(C_2H_4X)_2$ X=Cl, Br	S	[102]
1,7-$(C_4H_8X)_2$ X=Cl, Br, I	S	[102]
1-CH_2I	Dipole moment	[344]
1,7-$(C_4H_8I)_2$	S	[102]
Aryl derivatives		
1-Ph	C	[107]
1-*m*/*p*-C_6H_4Me	pK_a	[115]
1,7-(*p*-C_6H_4Me)$_2$	S	[116]
1-(C_6H_4-*p*-CN)	S, H, C, MS	[884]

Continued

Compound	Information	References
1-C_6H_4-*p*-CN-7-C_6H_4-*p*-NMeR R = C(O)Me, SO_2Me nonsteroidal progesterone receptor (PR) antagonists	S, H, C, binding assays	[872]
C_6H_3-1′,3′,5′-[$(C_6H_4)_2$-*p*-$C_2B_{10}H_{11})_3$	S, H, B, C, IR, MS, UV, fluorescence	[826]
1-C(O)OC_6H_4-*p*-CHO	S	[833]
1,7-[H_2N-C_6H_4-C≡C-$C_6H_4(CH_2)_n]_2$ *n* = 0,1	S, H, C, IR	[879]
cyclo-[-$CH_2C_6H_4CH_2$-$CB_{10}H_8$(9,10-Me_2)C-]$_4$ xylylene-linked carboracycle (FF)	S, H, B, C, MS	[123]
-[-C_6H_4-*p*-$CB_{10}H_{10}$C-(*p*-$C_6H_4)_n$-]- porous polymers for H_2 storage	S, H, B, IR, H_2 adsorption	[846]
1-*p*-HOC_6H_4-2-R-9-F R = H, *p*-HOC_6H_4OH, OH, CH_2OH, Br, I, CH_2CH═CH_2	S, H, B, C, estrogen receptor β binding affinity	[853]
$F_2C_2B_{10}H_9$-9-*p*-C_6H_4OH	S, H, B, C, estrogen receptor β binding affinity	[853]
1,7-(*p*-HOC_6H_4)2-9-R R = *n*-C_3H_7, *n*-C_4H_9	S, H, MS, estrogen receptor β selectivity in MCF-7 cell line	[860]
	S (from RMgX)	[95,98]
	S (Pd cross-coupling)	[96]
	S [UV photolysis of $Hg(C_2B_{10}H_{10})_2$]	[126]
	X	[127]
9,10-Ph_2	S	[97]
9,10-$(C_6H_4Me)_2$	S, H, B, C, MS	[128]
9-C_6H_4Me	S (from RMgX)	[95]
1,7-$(CH_2Ph)_2$	S	[77]
	E	[50]
9,10-$(CH_2Ph)_2$	S	[97]
1-CH_2R R = C_6H_6, MePh, *p*-MeC_6H_4Me	S	[130]
1-$C_6H_4NO_2$-7-R R = C(O)OMe, CH_2OH hydrophobic	S, H, C, MS, binding affinity	[638]
1-$CH_2C_6H_4$R-7-R′ R = H, NO_2, CN; R′ = OH, CH_2OH, $CH_2OSiMe_2CMe_3$ anti-androgenic activity	S, H, C, MS, transient transactivation assay	[641]
1-(*p*-C_6H_4-OH)-7-$(CH_2)_5CHMe_2$ incorporated into liposomes for BNCT	S, H, C, MS	[642]
1-(*p*-C_6H_4-OH)-7-[C_6H_4-*m*-O$(CH_2)_nNMe_2$]	S, estrogen receptor binding	[891]
1-$C_{13}O_2H_7$[C(O)OEt]-7-$CHMe_2$ 5,6-benzocoumarin	S, X, H, B, IR	[877]
1-[C(O)-$C_{13}O_2H_7$]-7-$CHMe_2$ 5,6-benzocoumarin	S, X, H, B, IR	[877]
1-CH$(C_6H_4$-*p*-$OH)_2$	S, H, C. S	[877]
Haloaryl derivatives		
1-[*p*-C_6F_4(*n*-C_4H_9)]-7-Ph	S, H, C, F, IR	[138]
p-$(RCB_{10}H_{10}C)_2C_6F_4$ R = Me, Ph (FF)	S, H, C, F, IR	[138]
p-[1,7-Ph$CB_{10}H_{10}$C]-C_6F_4-[1,2-$CB_{10}H_{10}$CH (FF)	S, H, C, F, IR	[138]
1-*p*-C_6H_4X X = Cl, Br, I	S	[139,140]
1-*p*-C_6H_4Br	S	[109]
1,4-[BrC_6H_4-$CB_{10}H_{10}$C]$_2C_6H_4$ (FF)	S, H, C, IR, MS	[107]
1,4-$C_6F_4(MeC_2B_{10}H_{10})_2$ (FF)	S	[141]

Compound	Information	References
1-C_6F_4Cl-7-R R = Me, Ph	S	[141]
(*m*/*p*-C_6H_4F)$HC_2B_{10}Cl_{10}$ (FF)	S, F	[142]
1-*p*-C_6H_4I	E	[114]
B-C_6F_5	S (high temp C_6F_6 + 1,7-$C_2B_{10}H_{12}$)	[767]
n-*p*-C_6H_4F *n* = 3, 4, 9	S	[143]
9-C_6H_4F	S (from RMgX)	[95]
1-(C_6H_3-3′-Me-4′-OH)-9-F X = F, Cl, Br	S	[893]
Alkenyl derivatives		
n-CH═CH_2, *n*-CH_2=CMe *n* = 3, 7, 9	MS (photoionization mass spectra)	[148]
1,7-H(Br_2C═CH)$C_2B_{10}H_2Me_8$ (FF)	S, H, B, C, MS	[153]
1-CF═CXY-7-Me X,Y = F, Cl, *n*-C_4H_9, Ph, CF_3, SC_4H_9, SPh, NEt_3	S, H, F	[154]
Alkynyl derivatives		
1,7-Me$CB_{10}H_2Me_8$C—C≡C— [C≡C—$CB_{10}H_2Me_8$C—C≡C-]$_2$-C≡C-$CB_{10}H_2Me_8$CMe (FF)	S, H, B, C, MS	[153]
p-[(C_8H_{17}-O)$_2C_6H_2$](C≡C-*p*-C_6H_4-$CB_{10}H_{10}$CH)$_2$	S, H, B, IR, UV	[122]
1,7-[H_2N-C_6H_4-C≡C-$C_6H_4(CH_2)_n$]$_2$ *n* = 0,1	S, H, C, IR	[879]
[{(F_3C)$_2$[$C_6H_3C_2$(═O)$_2$N]$_2$}$_2${C_6H_4-C≡C-C_6H_4-$(CH_2)_n$-$CB_{10}H_{10}$C-$(CH_2)_n$-C_6H_4-C≡C-C_6H_4}(C_6H_4-O-C_6H_4)]$_x$ *n* = 0, 1 polyimide films (FF)	S, H, C, IR	[879]
9-C≡C-C_4H_9	S	[96]
Alcohols and C- and B-hydroxy derivatives		
n-OH *n* = 1, 2, 4	pK_a	[176]
4-OH	pK_a	[177,178]
5-OH	pK_a	[178]
1,7-$(CH_2OH)_2$	MS (fragmentation patterns)	[813]
1-R R = H, OH, CH_2OH, $(CH_2)_3OH$	K_a association constant with β-cyclodextrin	[898]
1,7-R_2 R = H, OH, CH_2OH, $(CH_2)_3OH$	K_a association constant with β-cyclodextrin	[898]
1,7-H($HOCH_2$)$C_2B_{10}H_2Me_8$ (FF)	S, H, B, C, MS	[153]
1,7-R$CB_{10}H_2Me_8$C–C≡C—C≡C-$CB_{10}H_2Me_8$CR′ R, R′ = H, CH_2OH, C≡CH (FF)	S, H, B, C, MS	[153]
1,7-R_2 R = CMe_2OH, CMe(CF_3)OH, C(CF_3)$_2$OH, C(CF_3)(CF_2Cl)OH	S	[152]
1-R-7-C_6H_4-*m*/*p*-OH R = H, OH, CH_2OH, CH_2CH_2OH	Docking and scoring with estrogen receptor	[842]
1-*p*-HOC_6H_4-2-R-9-F R = H, *p*-HOC_6H_4OH, OH, CH_2OH, Br, I, CH_2CH═CH_2	S, H, B, C, estrogen receptor β binding affinity	[853]
$F_2C_2B_{10}H_9$-9-*p*-C_6H_4OH	S, H, B, C, estrogen receptor β binding affinity	[853]
1-$(CH_2)_3OH$-B-Me_8	S, H, B, C, MS	[105]
1,7-(*p*-$CH_2C_6H_4OH)_2$	S	[188,189]
[$HO(CH_2)_3$]$_2C_2B_{10}Me_8H_2$ (FF)	S, H, B, C, MS	[194]
1-C_6H_4-*m*/*p*-OH	pK_a; σ^- (inductive mechanism)	[190]

Continued

Compound	Information	References
n-p-C_6H_4OH *n* = 1, 2, 9	Partition coefficients (log *P*)]; Hansch-Fujita hydrophobic parameters; drug design	[669]
1,7-$(C_6H_4OH)_2$	Dipole moments	[192]
1,7-R_2 R = CHPhOH, CHMe OH	S	[78]
1-R-7-Me R = CH_2OH, $CH(OH)C_5H_5N$, $CH_2CH(OH)Ph$	S	[78]
1-R-7-Me R = CMe_2OH, CPh_2OH	S, H, IR	[193]
1-CHMeOH-7-Me	S	[214]
1-R-7-R′ R = $(CH_2)_2OH$, $C_2(CH_2CH_2OH)_2$; R′ = H, $CHMe_2$, $CMe{=}CH_2$	IR	[194]
1,7-$[CH(OH)Me]_2$	IR (variable *T*), Raman (variable *T*)	[43]
1-R-7-R′ R = H, R′ = OH, CH_2OH, NH_2; R = R′ = OH complexes with β-cyclodextrin	K_a (association constants)	[195]
1-(*m*/*p*-C_6H_4OMe)-7-R R = H, OH, $(CH_2)_nOH$ *n* = 1, 2, 3	S, H, MS	[196]
1-CH(OH)Ph	S, H, C, MS	[884]
1-Ph-7-$CH_2CH(OH)Me$	S, H, C, MS	[884]
(R)-1-(C_6H_4-p-CN)-7-CH(OH)Me	S(lipase TL-catalyzed asymmetric acetylation of 1-(C_6H_4-*p*-CN)-7-CH(OH)Me-1,7-$C_2B_{10}H_{10}$), H, C, MS, progesterone receptor activity	[884]
1-{*cyclo*-[CHCH═CHC(O)CH_2CH_2]}-2-CH_2OH hydrophobic cage; binds to androgen receptor and shows anti-androgenic activity	S	[672]
1-C(OH)C≡CMe_2(O)OR′ -7-R R = H, $CHMe_2$, CMe_2Et; R′ = CMe_3, CMe_2Et, $CMe_2(CH_2)_2Me$ peroxy alcohols	S, IR	[197]
1-C(OH)PhC≡CMe_2OOR R = CMe_3, CMe_2Et, $CMe_2(CH_2)_2Me$ peroxy alcohol	S, H, IR	[812]
1,7-{CH(OH)-[2,2]paracyclophane}$_2$	S, IR	[198]
9,10-$(CH_2CH_2OH)_2$	S, IR	[200]
9-$CHMe(CH_2)_2C(O)OH$	S	[201]
9-CH(OH)Ph	S	[203]
9-$(CH_2)_nCH(OH)(C_5H_4)FeCp$ *n* = 0, 1	S, H, B, IR	[885]
9-$CH_2CR(OH)(C_5H_4)FeCp$ R = H, Me	S, H, B, IR	[885]
Aldehydes		
1-C(O)H	S, IR	[206]
	S, IR (actual spectrum)	[207]
	S	[208]
1-$C(O)OC_6H_4$-*p*-CHO	S	[833]
1,7-$[C(O)H]_2$	S	[208,210]
1-C(O)H-7-Me	S	[193]
1-$CH_2C(O)H$	S	[211]
1-$CH(OEt)_2$ acetaldehyde diethyl acetal	S	[211]
1-$CH_2C(O)H$-7-Me	S	[193,212]
Ketones		
1-C(O)Me-7-Me	S	[214]
	IR (actual spectrum)	[215]

Compound	Information	References
1-C(O)CH_2Br-7-Me	S, IR (actual spectrum)	[215]
1,7-R_2 R═C(O)Me, C(O)Ph	S	[78]
$PhCB_{10}H_{10}C$-CHPhCH_2C(O)-$CB_{10}H_{10}C$-Ph (FF)	S	[78]
1,7-[1,2-$RCB_{10}H_{10}CC(O)]_2C_2B_{10}H_{10}$ R=H, Me (FF)	S, IR, MS	[129]
1,7-[C(O)CH═CHR]$_2$ R=Ph, *p*-$MeOC_6H_4$, *p*-FC_6H_4, 2-furyl, 2-furylvinyl) α,β-unsaturated ketones	S	[216]
9-$CH_2C_6H_4$C(O)Ph	S	[97]
9-CH_2-*p*-C_6H_4C(O)Ph	S, B	[220]
9,10-[CH_2C(O)Ph]$_2$	S	[200]
9-$(CH_2)_n$C(O)(C_5H_4)FeCp *n*=0, 1	S, H, B, IR	[885]
Carboxylic acids		
1-C(O)OH-7-C_6H_4-*m*-F	Transthyretin (TTR) and COX (cyclooxygenase) inhibition assays	[229]
1-$(CH_2)_n$C(O)OH *n*=0,1	pK_a, induction constants	[231]
1-CH_2C(O)OH	S	[232]
	pK_a, E (half-neutralization potential)	[226]
1,7-[CH_2C(O)OH]$_2$	MS (fragmentation patterns)	[813]
1-C(O)OH-7-R R=H, Me	S, I (actual spectrum)	[233]
1-C(O)OH-7-Me	S, pK_a	[75]
1-C(O)OH-7-Ph	S	[110]
1,7-[*p*-$CH_2C_6H_4$C(O)OH]$_2$	S	[189]
1,7-[*p*-C_6H_4C(O)OH]$_2$	S	[116]
1,7-[C_6H_4C(O)OH]$_2$	Dipole moments	[192]
1-C(O)OH-7-N(boc)NH(boc) boc=*tert*-butyloxycarbonyl]hydrazine	S, H, B, C, MS	[268]
B-C(O)OH	S	[780]
B,B′-[C(O)OH]$_2$	S	[780]
1,7-[C(O)OH]$_2$ N- and P-containing salts	S, H, IR	[238]
Esters and acyl halides		
1-C(O)Cl-9-I	S, H, B, C	[890]
1,7-[C(O)Cl]$_2$	S	[75,239]
1-C(O)Cl-7-Ph	S	[110]
1-C(O)OH-7-R-9-I R=H, C(O)OH	S, H, B, IR	[862]
1-C(O)OH-7-R-9,10-I_2 R=H, C(O)OH	S, H, B, IR	[862]
1-C(O)Cl-7-C(O)NHPh	S, reaction kinetics	[242]
1-CH_2C(O)OMe-7-R R=H, CH_2C(O)OMe	S	[182]
1-C(O)OMe-7-C_6H_4-*m*-F	Transthyretin (TTR) and COX (cyclooxygenase) inhibition assays	[229]
$HCB_{10}H_{10}C$-C(O)-OO-CMe_2-C≡C-CMe_2-OO-C(O)-$CB_{10}H_{10}CH$ peroxy ester (FF)	S, $\Delta H_{formation}$, $\Delta H_{combustion}$	[247]
1-CH_2NH-CH[C(O)OMe]CH_2CHMe_2	S, H, C, MS	[205]
1-CH═NCH[C(O)OMe]CH_2CHMe_2	S, H, C, MS	[205]

Continued

Compound	Information	References
(R)-1-Ph-7-CHMeOAc	S(lipase TL-catalyzed asymmetric acetylation of 1-Ph-7-CH(OH)Me-1,7-$C_2B_{10}H_{10}$), H, C, MS, progesterone receptor activity	[884]
1-Ph-7-[*N*-(2-carboxy-4,5-dichlorobenzoyl)-(-)-1,2-camphorsultam]	S, X, H, C, MS	[884]
1-R-7-R′ R = $CH_2C(O)OX$, $C_2(CH_2C(O)OX)_2$; R′ = H, $CHMe_2$, $CMe{=}CH_2$; X = H, Cl	IR	[194]
1,7-$[CMe_2OC(O)Me]_2$	S	[152]
1-C(O)Me-7-R R = terpene, sterol, plant phenol, oxime	S, H, IR, UV	[808]
1-$C(O)O(CH_2)_nOOR$ R = CMe_3, CMe_2Et; *n* = 1, 2 peroxy esters	S	[252]
1-C(O)OH *tert*-butyl polyesters	Enthalpy of combustion, enthalpy of formation, heat capacity temperature dependence	[807]
1-$C(O)OOCMe_2C{\equiv}CH$-7-R [R = H, $CHMe_2$ peroxy alkynes	S, heat capacity temperature dependence, $\Delta H_{combustion}$	[246]
1-$[C(O)OOCMe_2C{\equiv}C\text{-}CMe_2OOCMe_3]$ peroxy alkyne	S, heat capacity temperature dependence, $\Delta H_{combustion}$	[246]
$HCB_{10}H_{10}C\text{-}C(O)\text{-}OO\text{-}CMe_2\text{-}C{\equiv}C\text{-}CMe_2\text{-}OO\text{-}C(O)\text{-}CB_{10}H_{10}CH$ peroxy ester (FF)	S, $\Delta H_{formation}$, $\Delta H_{combustion}$	[247]
1-C(O)OOR R = CMe_3, CMe_2Et peroxy esters	S	[782]
1-$C(O)OOCMe_3$ peroxy ester	S	[783]
1-OOR-7-R′ R = CMe_3, CH_2Ph, H; R′ = Me, $CHMe_2$, $CHMe{=}CH_2$ peroxides	S	[248]
1-C(O)OOR R = CMe_3, CMe_2Et, C(O)Me, CH_2Ph peroxides	S	[249]
1-C(O)OOR-7-C(O)OOH R = CMe_3, CMe_2Et peroxides	S	250
1,7-$[C(O)OOR]_2$ R = Me, Ph peroxides	S	[250]
1-$C(OH)C{\equiv}CMe_2(O)OR'$ -7-R R = H, $CHMe_2$, CMe_2Et; R′ = CMe_3, CMe_2Et, $CMe_2(CH_2)_2Me$ peroxy alcohols	S, IR	[197]
1-$[CH_2C_6H_4$-*p*-$OC(O)Me]$	S	[251]
1-$[(C_6H_4)_2$-*p*-$OC(O)Me]$	S	[251]
1,7-$[C(O)O(CH_2)_nOOR]_2$ R = CMe_3, CMe_2Et; *n* = 1, 2 peroxy esters	S	[252]
1,7-$[CH_2(O)OCR]_2$ R = Et, Me_2CH, Ph	S	[243]
1,7-$[C(O)OR]_2$ R = $CH_2CH{=}CH_2$, $CH_2C{\equiv}CH$	S	[253]
B-C(O)OR R = Me, $SiMe_3$,Cl	S	[780]
B,B′-$[C(O)OR]_2$ R = Me, $SiMe_3$,Cl	S	[780]
n-OC(O)Me *n* = 2, 3, 4, 9	S	[178]
B,B′-$[OC(O)Me]_2$	S	[178]
9,10-$[CH_2C(O)Cl]_2$	S	[200]
Ethers, epoxides, and peroxides		
1-$CH_2OCH_2CH{=}CH_2$	S	[254]
1,7-$(CH_2OCH_2CH{=}CH_2)_2$	S	[254]
1-R-7-R′ R, R′ = $CH_2OC_4H_9$, CH_2OCH_2Ph	S	[255]
1-*p*-C_6H_4OMe	S	[139]
$(Br\text{-}CB_{10}H_{10}C\text{-}CH_2)_2O$ (FF)	S	[102]
1-$[CH_2(cyclo\text{-}CHCH_2O\text{-})]$-7-Me	S	[78]

Compound	Information	References
B-$(CH_2)_2$Si$(OOR)_3$ R = CMe_3,CMe_2Et, 2-cyclohexylisopropyl peroxides	S	[258]
1-{[*bicyclo*-C_4(OH)O-O_2CMe_2]-[*cyclo*-$C_3O_2CMe_2$]} L-mannofuranose aldose for BNCT	S, X	[806]
Nitro and nitroso derivatives and nitrates		
1-*p*-$C_6H_4NO_2$	S	[139,260]
1,7-[C(O)OC_6H_4-*o*-NO_2]$_2$	S	[261]
1,7-($SCH_2C_6H_4$-*p*-NO_2)$_2$	S, H, C, IR, MS	[897]
Amines and imines		
1-NH_2-7-R R = H, Ph	S	[263]
1-$CH_2CH(NH_2)C(O)OH$ alanine enantiomers	S, H, B, C, IR, optical rotation	[185]
1-*p*-$C_6H_4NH_2$	S	[140]
1-*m*/*p*-$C_6H_4NH_2$	pK_a, σ^- (inductive mechanism)	[190]
1,7-[C(O)O-p-$C_6H_4NH_2$]$_2$ aminophenyl oxycarbonyl	S	[266]
1,7-[C(O)NH-p-$C_6H_4NH_2$]$_2$ aminophenyl carbamoyl	S	[266]
1-OC_6H_3(OR)CH═N$(CH_2)_2NC_6H_3$Me R = Me, Et Schiff bases	S, H, I	[267]
1-N(boc)NH(boc)-7-C(O)OH boc = *tert*-butyloxycarbonyl]hydrazine	S, H, B, C, MS	[268]
1-C(O)OC_6H_4-*p*-HC═NR R = *n*-$C_{13}H_{37}$, Ph, C_6H_4Ph, naphthyl, *p*-C_6H_4Me, $C_6H_4C(O)OH$, $C_6H_4C(O)OEt$, CH(adamantyl)Me, L-CH($CHMe_2$)C(O)OMe, C_6H_4OH, C_6H_4Oph	S	[833]
1-$H_2NSO_2NHCH_2$	X(complex with carbonic anhydride CAII), *in vitro* inhibition in carbonic anhydrase	[850]
1,7-[$H_2NSO_2NHCH_2$]$_2$	*In vitro* inhibition in carbonic anhydrase	[850]
2-NPh_2	S, IR	[273]
1-$(CH_2)_3NH_2$-B-Me_8	S, H, B, C, MS	[105]
1,7-Me_2-3-NH_2	S	[275]
9,10-[$C_6H_4NMe_2$]$_2$	S, H, B, C, MS	[128]
[$H_2N(CH_2)_3$]$HC_2B_{10}Me_8H_2$ (FF)	S, H, B, C, MS	[194]
[$ClNH_3(CH_2)_n$]$_2C_2B_{10}Me_8H_2$ *n* = 3, 4 (FF)	S, H, B, C, MS	[194]
1-$(CH_2)_3$OCH[CH_2OCH(CH_2OH)$_2$]$_2$-7-$(CH_2)_2C_4H_5$[C(O)OH]NH_2 water-soluble amino acid cascade polyol for BNCT	S, H, C, IR	[277]
1,7-(C_6H_4-*p*-$C_6H_4NH_2$)$_2$	S, H, C, IR, MS	[897]
1,7-($SCH_2C_6H_4$-*p*-NH_2)$_2$	S, H, C, IR, MS	[897]
Heterocyclic amines		
5,10,15,20-(*p*-$C_6H_4NH_2$)$_4$ porphyrin derivatives	S	[276]
Thymidine derivatives for BNCT (substrates for human thymidine kinase I)		[804,805]
Other thymidine-pyrimidine nucleoside analogues	S, cell uptake and biodistribution studies	[892]
Ethylene oxide-modified 3-*m*-carboranyl thymidine derivatives for BNCT	S	[696]
NC_5H_3-2,6-($CB_{10}H_{10}CH$)$_2$ lutidine (FF)	S, H, B, C, MS	[123]
Cyclo-[−(2,6-NC_5H_3)-CH_2-$CB_{10}H_{10}C$-CH_2-]$_2$ lutylidine-linked carboracycle (FF)	S, X, H, B, C, MS	[123]

Continued

Compound	Information	References
Cyclo-[-2,6-(O)NC_5H_3-CH_2-$CB_{10}H_{10}$C-CH_2-]$_2$ lutylidine *N*-oxide-linked carboracycle (FF)	S, H, B, C, MS	[123]
1,7-[C(O)NHCHRCH_2X]$_2$ R = $CHMe_2$, CH_2Ph; X = Br, Cl oxazolinyl pincer ligands	S, X, H, B, C, IR, MS	[823]
ClM[1,7-*cyclo*-C═NCRR′CH_2O)$_2C_2B_{10}H_{10}$ M = Ni, Pd; R = H, Ph; R′ = H, $CHMe_2$, CH_2Ph 2(N → M), B(2) → Rh oxazolinyl pincer complexes (FF)	S, H, B, C, IR, MS	[823]
Indomethacin-$C_2B_{10}H_{11}$ COX inhibition, enzyme selectivity (FF)	S, X, H, B, C, MS, IR	[832]
1,7-(C_6H_4-*p*-$NC_{12}H_8$)$_2$ carbazolyl wide band gap; blue phosphorescence	S, H, C, UV, photoluminescence spectra, DSC, E, transient photocurrent measurements (charge mobility)	[836]
(porphyrin)(9-CH_2CH_2CMe-$C_2B_{10}H_{11}$)$_4$ (FF)	S, H, cytotoxicity	[269]
9-S-*cyclo*-C_4H_2(═O)$_2$N-C_6H4-*p*-(porphyrin)Ph_3 *N*-malemido	S, H, B, MS	[876]
9-(2′,5′-diazabicyclo[2′.2′.2′]oct-2-ene) derivatives	S, X, H, MS	[282]
9-CH_2-[C_5H(CN)Ph(*p*-tolyl)N] (2 isomers) pyridyl	S	[280]
9-R R = dioxolylthienyl, methylindolyl, 2′/3′-pyridyl	S, H, B, MS	[281]
9-pyridinium-*nido*-$C_2B_9H_{12}$	S	[180]
9-C(O)-*cyclo*-N_4C-Ph tetrazole	S, H, B, IR	[844]
9-CH_2-C(O)-*cyclo*-N_4C-Ph tetrazole	S, H, B, IR	[844]
9-*cyclo*-[C═N—N═CPh—`O—] oxadiazole	S, X, H, B, IR	[844]
9-CH_2-*cyclo*-[C═N-N═CPh—O—] oxadiazole	S, H, B, IR	[844]
9-CH_2-*cyclo*-C_2N_3-4′-Ph-5′-$C_6H_3Cl_2$ 1,2,4-triazole	S, H, B, IR	[844]
9-CH_2-C_4HN_2($N_2C_3Me_2H$)$_2$ pyridazine, pyrazoyl supramolecular assembly with tetrachlorohydroquinone	X	[859]
Amides and imides		
[—C(O)—$CB_{10}H_{10}$C—C(O)NH—C_6H_4-*p*-NH—]$_n$ polyamide (FF)	D, IR, DTA	[283]
1,7-(maleamidocarboxylic acid}$_2$	S	[284]
1,7-(maleamide)$_2$	S, IR	[284]
1-[*cyclo*-C═N—O—CR═CH—] R = Ph, C(O)OMe isoxazoles, isoxazolines	S	[286]
1-(CH_2)$_2$NHC(O)CH═CH—C_5H_4N nicotinamide derivative increases potency of small molecule inhibitors of nicotinamide phosphobosyltransferase (Nampt)	S, H, B. C, MS	[830]
1-(*bicyclo*-C_7NSH_4)-9-R benzothiazole R = H, I, NHC(O)CF_3, NH_2	S, H, B, C, MS(NH_2)	[890]
1-C(O)Cl-9-I	S, H, B, C	[890]
1-(*bicyclo*-C_7NSH_3OH)-9-NH_2 benzothiazole	S, H, B, C, MS	[890]
—[—C_6H_4-*p*-CH_2S-$CB_{10}H_{10}$C-S$CH_2C_6H_4$-*p*-(*bicyclo*-$C_8H_3O_2N$) —O—(*bicyclo*-$C_8H_3O_2N$)—]— polyimide	S, TGA, XRD, IR	[897]
9-CH_2-*cyclo*[CHC(R)═N—N═C(R)CH_2] R = CH_2-3′,6′-di(indazolyl)-4,5-dihydropyridazine	S([4 + 2] cycloaddition), X, MS	[816]
9-CH_2-*cyclo*-(3,6-R_2-4,5-pyridazine) R = di(indazolyl), 3′,5′-dimethylpyrazoyl, 4-methylimidazoyl, Ph, 3-pyridyl, 2-pyridyl	S([4 + 2] cycloaddition), X(Ph)	[816]
1-CHMeEt-2-C_6H_4-*m*/*p*-OCH_2C(O)NH-C_6H_3(OH)-B(pin) acetanilides	S, H, C, MS, inhibition of hypoxia-induced HIF-1 transcriptional activity	[896]

Compound	Information	References
Azides		
1-$(CH_2)_3N_3$-B-Me_8	S, H, B, C, MS	[105]
$[N_3(CH_2)_n]_2C_2B_{10}Me_8H_2$ $n=3$, 4 (FF)	S, H, B, C, MS	[194]
$[N_3(CH_2)_3]HC_2B_{10}Me_8H_2$ (FF)	S, H, B, C, MS	[194]
1,7-(CH_2-*cyclo*-$N_3C_2RH)_2$ triazolylmethyl R = Ph, H, C_5H_{11}	S, H, B, IR	[834]
Nitriles and isonitriles		
$[NC(CH_2)_n]_2C_2B_{10}Me_8H_2$ $n=3$, 4 (FF)	S, H, B, C, MS	[194]
n-CN $n=2$, 4	S (isomerization of 1,2-$C_2B_{10}H_{11}$-3-CN)	[177]
9-[4-S-1′,2′-$C_6H_3(CN)_2$]	S (nucleophilic substitution of NO_2), H, IR	[295]
9-*p*-C_6H_4-O-$C_6H_3(CN)_2$	S	[257]
Ureas		
Urea-based glutamate carboxypeptidase II inhibitors		[899]
Phosphorus derivatives		
1-PMe(OEt)-7-R R = H, Me, CH_2═CMe, Ph	S	[297]
1-[PMe(OEt)═N-C_6H_4-*p*-NO_2]-7-R R = H, Me, CH_2═CMe, Ph)	S	[297]
1-PMe(OEt)R• R = $OCMe_3$, Me phosphoranyl radicals	ESR	[298]
1-$(MePh_2P)^+I^-$ selective targeting of mitochondria for BNCT	S, H, B, C, P, MS	[299]
1-OP(O-C_6H_3-2′,6′-$Me_2)_2$ phosphite Suzuki-Miyaura Pd-catalyzed cross-coupling with aryl bromides	S, H, B	[818]
1,7-{P*Br[$N(CHMe_2)_2$}$_2$ chiral	S, X, H, B, C, P, IR, MS	[302]
$(HCB_{10}H_{10}C\text{-}CH_2O)PCl_2$ phosphorodichloridite (FF)	S	[182]
$(HCB_{10}H_{10}C\text{-}CH_2O)_2PCl$ phosphorodichloridate (FF)	S	[182]
1,7-[P(OMe)(NR_2)]$_2$ R = $CHMe_2$, Me precursors to 1,2-glycophosphonates via condensation with galactose	S, H, B, C, P, MS, IR	[811]
1,7-{P(X)[OCH_2-*cyclo*-$C_5H_5(OH)_4O]_2\}_2$ X = O,S water-soluble glycophosphonates for BNCT	S, H, B, C, P, MS, IR	[305]
	S	[307]
9-$OPO_2(C_{10}H_6)_2$ phosphite ligands for Rh-catalyzed asymmetric hydrogenation of dimethyl itaconite	S, H, B, P	[793]
1-O[PN(Ph)NC_5H_9] diamidophosphite Pd-catalyzed allylic substitution reactions with C-, S-, and N-nucleophiles with low enantioselectvity	S, B, C, P, MS	[810]
Cis/*trans*-$Cl_2Pt(Ph_2P\text{-}9\text{-}C_2B_{10}H_{11})_2$	S, X(*trans*), H, B, P, IR	[837]
$Rh\left[Ph_{=}P(CH_2)_2S-9-1,7-C_2B_{10}H_{11}\right]_2^-$	S, X, H, B, C, MS	[849]
$Rh\left[Ph_{=}P(CH_2)_2S-9-1,7-C_2B_{10}H_{11}\right]_2^-$ $Rh\left[Ph_2P(CH_2)_3S-CB_{11}H_{11}\right]_2^-$	S, X, H, B, C, MS	[849]
Sulfur derivatives		
1-SH-*n*-X $n=9$, 10; X = Cl, Br	S, H, B, pK_a	[308]
n-SH $n=1$, 4, 9	MS, pK_a, dipole moment	[176]
9-SH	S, X, thermal isomerization	[895]
1,7-$(SMe)_2$-9,10-X_2 X = H, Br	S, B (antipodal shielding), C	[20]
1-$[S(O)Ph]_2$-7-Ph	S, IR	[311]
1-SH-7-R R = H, Me	S	[312]

Continued

Compound	Information	References
1-CMe═S	S, H, B, C	[313]
1-R R═C(═S)SMe, CH_2SH	S, X, H, B, C, MS	[314]
1-(terpyridine)PtSCH_2-$C_2B_{10}H_{11}^+$ $OSO_2CF_3^-$ (FF)	S, X, H, B(2d), C, MS	[314]
1-NH—C(═S)—NHR R = Ph, C_5H_4N, *cycle*, 1′-(1′,7′-$C_2B_{10}H_{11}$) (FF)	S, H, B. C, IR, MS	[845]
$Rh\left[Ph_{=}P(CH_2)_3S-9-1,7-C_2B_{10}H_{11}\right]_2^-$ (FF)	S, X, H, B, C, MS	[849]
[—SC_4H_2—$CB_{10}H_{10}C$—C_4H_2S—]$_n$[*cycle*-SC_4H_2(3,4-OCH_2CH_2O)]$_m$ (FF) conjugated carborane-thiophene copolymer with 3,4-ethylene-dioxythiophene	S(electrochemical), H, IR, E, UV, electro-optical spectra	[856]
Cis/*trans*-1-CH═CH-C_4HBr_2S thiophene	S, H, B, C, MS	[875]
$(C_2B_{10}H_{10})_2$\{1,7-*cyclo*-[$S(CH_2)_nS$-}$_2$ *n* = 6–8 (FF)	S, X(*n* = 7), H, B	[86]
1-SCl-7-SOEt	S	[315]
1-CPhH($OSO_3C_6H_4Me$)-7-C_6H_4R R = H, CF_3, Me, OMe, NMe_2 tosylates	S, rate constants, electronic effects of substituents	[320]
1-benzyl *p*-toluenesulfonates tosylates	Hydrolysis kinetics	[322]
1-(*bicyclo*-C_7NSH_4)-9-R benzothiazole R = H, I, $NHC(O)CF_3$, NH_2	S, H, B, C, MS(NH_2)	[890]
1-(*bicyclo*-C_7NSH_3OMe)-9-R benzothiazole R = H, I, $NHC(O)CF_3$, NH_2	S, H, B, C, MS	[890]
1-(*bicyclo*-C_7NSH_3OH)-9-NH_2 benzothiazole	S, H, B, C, MS	[890]
9-$SCH_2C(O)OH$	MS, pK_a, dipole moment	[176]
9-X X = SH, SMe	X-ray photoelectron	[309]
9,10-SR_2 R = H, Me	S (electrophilic sulfuration with S_2Cl_2), H, B	[326]
	S	[331]
9,10-*cyclo*-[-S-CPhH-S-]	S, H, B	[326]
9,10-*cyclo*-[-S-CRR′-S-] R = H, Me; R′ = Ph, Me heteroacetals	S	[331]
(—S—$CB_{10}H_{10}C$—S—)$_n$ polydisulfide (FF)	S	[334]
Fluoro derivatives		
1,7-R_2 R = CMe(CF_3)OH, $C(CF_3)_2OH$, $C(CF_3)(CF_2Cl)OH$	S	[152]
1-R-9-F R = H, Me	S	[335]
1-CF═CFC(O)OH-7-Me	S	[336]
1-CF═CFR-7-Me R = H, F	S	[336]
1-*p*-HOC_6H_4-2-R-9-F R = H, *p*-HOC_6H_4OH, OH, CH_2OH, Br, I, $CH_2CH═CH_2$ (FF)	S, H, B, C, estrogen receptor β binding affinity	[853]
$F_2C_2B_{10}H_9$-9-*p*-C_6H_4OH (FF)	S, H, B, C, estrogen receptor β binding affinity	[853]
B-$CF(CF_3)$-C•(CF_2CF_3)[$CF(CF_3)_2$] radical	ESR	[341]
Chloro derivatives		
1-Cl-7-Me	H, B, IR (substituent effects)	[22,23]
1-Cl-7-R R = H, Me	^{35}Cl NQR	[345]
1,7-Me_2-5,12-Cl_2	S (thermal isomerization of 1,7-Me_2-9,12-Cl_2-1,2-$C_2B_{10}H_{12}$), X	[349]
3,9,10-Cl_3	H, B, IR (substituent effects)	[23]
	H (C-H shift, coupling constants)	[24]
	H	[350]

Compound	Information	References
n,9,10-Cl_3 *n*=3, 4	S	[351]
3, 8, 9, 10-Cl_4	H (C-H shift, coupling constants)	[24]
	H	[350]
n-Cl *n*=4, 5, 9	S	[352]
9-Cl	S	[338,352–357]
	Dipole moment	[363,364]
9-ClPh^+ BF_4^-	S, H	[365]
9-ClR^+ BF_4^- R=Ph, C_6H_4F	S	[145]
10-Cl	H (C-H shift, coupling constants)	[24]
1-Me-9-Cl	S	[354]
	IR (C-H intensity)	[39]
1-Me-7-R-9-Cl R=H, Me	H	[366]
1-R-9,10-Cl_2 R=H, Me	IR (C-H intensity)	[39]
9,10-Cl_2	Dipole moment	[363,364]
1-Me-7-R-9,10-Cl_2 R=H, Me	H	[366]
1-R-9,10-Cl_2 R=H, Me	^{35}Cl NQR	[361]
9,10-Cl_2	H (C-H shift, coupling constants)	[24]
1-Me-9,10-Cl_2	S	[354]
1,7-Me_2-9,10-Cl_2	S	[354]
4,9,10-Cl_3	Dipole moment	[364]
4,8,9,10-Cl_4	Dipole moment	[364]
$H_2C_2B_{10}Cl_8Br_2$ (FF)	S	[369]
$H_2C_2B_{10}Cl_{10}$ (FF)	S	[371]
	IR (H-bonding with bases; solvent effects)	[373]
	Dipole moment	[364]
(*m*/*p*-C_6H_4F)$HC_2B_{10}Cl_{10}$ (FF)	S, F	[142]
$R_2C_2B_{10}Cl_{10}$·L R=H, D; L=dioxane, Ph_3PO, pyridine, DMSO (FF)	IR, Raman (C-H—X bonds)	[375]
Bromo derivatives		
1-Br	Dipole moment	[344]
1-Br-7-Me	S	[378]
	H, B, IR (substituent effects)	[22]
1-Me-7-R-9-Br R=H, Me	H	[366]
1-Me-7-R-9,10-Br_2 R=H, Me	H	[366]
1,7-Me_2-7-R-9,10-Br_2 R=H, Me	S	[369]
1,7-Me_2-9,10-Br_2 R=H, Me	S, B(antipodal shielding), C	[20]
1-Me-9-Br	S	[354]
$C_2B_{10}H_{11}$-9-BrPh^+ phenylbromonium salt (FF)	S	[180]
1-*p*-HOC_6H_4-2-Br-9-F	S, H, B, C, estrogen receptor β binding affinity	[853]

Continued

Compound	Information	References
9-Br	H	[350]
	Dipole moment	[363,364]
	He photoelectron spectra	[360]
9-BrR^+ BF_4^- R=Ph, C_6H_4F	S	[145]
1,7-Br_2	Dipole moment	[68]
B-Br_2	S	[370]
9,10-Br_2	Dipole moment	[363,364]
1-Me-9,10-Br_2	S	[354]
	IR (C-H intensity)	[39]
$H_2C_2B_{10}Br_3H_7$ (FF)	Dipole moment	[363,364]
$H_2C_2B_{10}Br_3H_7$ (two isomers) (FF)	S	[354]
1-Me-4,9,*n*-Br_3 *n*=10, 12	S, X(*n*=12)	[386]
$MeHC_2B_{10}Br_3H_7$ (FF)	S	[351,354]
$H_2C_2B_{10}Br_4H_6$ (FF)	S	[355]
	IR (actual spectrum)	[39]
	Dipole moment	[363,364]
	E	[50]
4,8,9,10-Br_4	Dipole moment	[364]
$MeHC_2B_{10}Br_4H_6$ (FF)	S	[351]
$MeHC_2B_{10}Br_5H_5$ (FF)	IR (C-H intensity)	[39]
$H_2C_2B_{10}Br_6H_4$ (FF)	S	[355]
	IR (C-H intensity)	[39]
	IR (actual spectrum)	[39]
$H_2C_2B_{10}Cl_8Br_2$ (FF)	S	[369]
$H_2C_2B_{10}Br_{10}$ (FF)	Dipole moment	[363,364]
Iodo derivatives		
1-I	Dipole moment	[344]
n-I *n*=2, 9	^{75}Br labeling using Pd-catalyzed H exchange for BNCT	[387]
1,7-I_2	S	[347,378]
1-I-7-Ph	S	[110]
$[RR'C_2B_{10}H_9$-9-I$]^{-\cdot}$(FF) radical anions (R, R′=H, Me) (FF)	MS (electron resonance capture mass spectra)	[72]
9-I	He photoelectron spectra	[360]
	^{127}I NQR	[391]
	Dipole moment	[363,364]
9-^{125}I	S (radiolabeling via Pd-catalyzed isotopic exchange)	[392]
1-Me-7-R-9-I R=H, Me	H	[366]
9-IR_2 R=Cl, O_2CCF_3	S	[393]

Compound	Information	References
9-IR^+ R = Ph, 4-anisyl, 4-C_6H_4F, 3-$O_2NC_6H_4$, 2,4,6-$C_6H_2Me_3$ aryliodonium salts	S	[396]
9-IR^+ R = OCH_2Ph, N_3,N = PPh_3, NH_2, *p*-$O_2SC_6H_4Me$, O_2SPh, NCS, SCN, NHMe	S	[397]
9,10-I_2	H	[94,350]
	B	[94,367]
	Dipole moment	[363,364]
1-Me-7-R-9,10-I_2 R = H, Me	H	[366]
1-Me-9,10-I_2	S	[355]
***Exo*-Polyhedral Main-Group Metal and Metalloid Element Derivatives**		
Magnesium and calcium		
[—O(O)CR-NH(O)C-$CB_{10}H_{10}$C-C(O)NHR-C(O)O-M^{2+}–]$_n$ M = Mg, Ca; R = CHMe, $(CH_2)_m$, *m* = 2, 6, 7, 9 oligomeric salts (FF)	S	[402]
[—1,7-O(O)C-$CB_{10}H_{10}$-C(O)O-M^{2+}—]$_n$ M = Mg, Ca, oligomeric salts (FF)	S, COND, thermal and electrophysical properties	[403,404]
Thallium		
$Tl[OC(O)O]_2^{2+}$ $[Me_2C_2B_{10}H_9]_2^{2-}$ (FF)	S	[407]
1-$TlClC_4H_9$Cl-7-R R = H, Ph	S	[408]
1-R-7-R′-B-$Tl(O_2CCF_3)$ R, R′ = H, Me	S, kinetics of thallation	[409]
1,7-Me_2-9-$Tl(O_2CCF_3)_2$	S	[410]
1,7-R_2-9-$TlSn\{CH[MeC(O)O]_2\}_2Br_2$ R = H, Me	S	[411]
1,7-RR′-B-$Tl(O_2CCF_3)$ R, R′ = H, Me, Ph	S	[413]
9-Tl(2,2′-bipyridine)$[O(O)CCF_3]_2$	X	[418]
Silicon		
$(1,7\text{-}C_2B_{10}H_{11})_2SiMe_2$ (FF)	S	[422]
$O[SiMe_2CB_{10}H_{10}CSiMe_3]_2$ (FF)	S	[420]
1-$SiMe_2$OR R = H, Me	S	[420]
1-$OSiR_3$-7-R R = H, $OSiR_3$ siloxanes	IR (detailed study)	[427]
1-*cyclo*-$[(CH_2)_3SiMe]$-7-Me	S	[428]
$[1\text{-Me-}1,7\text{-}C_2B_{10}H_{10}]_2$[*cyclo*-$SiMe(CH_2)_3$] (FF)	S	[428]
1-CH_2SiMe_2OMe-7-R R = H, CH_2SiMe_2OMe	S	[429,430]
1-$SiMe_2$R-7-SiMeR′R″ R = H, OMe, OEt; R′ = Me, $(CH_2)_2CF_3$; R″ = H, Cl, OMe	S	[431]
1-SiMeRR′-7-SiMeR″OSiMeRR′ R, R″ = Me, Ph, $(CH_2)_2CF_3$; R′ = H, OMe, OEt,OH	S	[432]
1-$CH_2SiMe_2OSiMe_3$-7-Me	S	[433]
1-C(OSiMe_3)═P$SiMe_3$	S, H, C, P	[303]
1,7-$\{O[SiMe_2]_2CH{=}CH_2\}_2$	S	[436]
1,7-$[(CH_2)_3SiMe_2Cl]_2$	S	[437]
1,7-$[(CH_2)_3SiMe_2(OMe)]_2$	S	[437]
1,7-$[(SiMe_2O)_2(SiMe_3)]_2$-9-Cl	S, H	[438]
1,7-$[(SiMe_2R]_2$ R = H, OMe, OEt	S	[439]

Continued

Compound	Information	References
1,7-[$SiMe_2OR]_2$ R = $SiMe_2Cl$, $SiMePhCl$, $Si(CH{=}CH_2)MeCl$, $SiMe_2H$, $SiMe_2(OMe)$), $SiHMeOC(O)Me$, $SiMe_2OC(O)Me$ disiloxanyl	S	[440]
1,7-R_2 R = $SiMe_2OEt$, $SiMe_2OMe$, $SiMe_2OPh$	S	[422]
1,7-[$SiR_2(OMe)]_2$ R = Me, Et	S	[441]
1,7-[$SiMe_2(OH)]_2$	S, reaction mechanisms	[441]
1,7-[$SiMe_2OEt]_2$	S	[442]
1,7-[$SiMe_2$-O-$SiMe_2$-R]$_2$ R = $CH{=}CH_2$, C≡CH hydrosilylation via Karstedt catalysis → elastomeric network polymers	DSC, TGA	[443]
1,7-[$CH_2SiMe_2Cl]_2$	S (thermal isomerization of *o*-carboranyl isomer)	[444]
1,7-[$SiMe_2Cl]_2$	S	[445]
1,7-($SiPh_2R)_2$ R = Cl, Me	S	[446]
1,7-($SiPhMe_2)_2$	S	[446]
{($SiPh_2]_2C(=CH_2)$-1,7-$C_2B_{10}H_{11}\}_2$ (FF)	S	[447]
1,7-{[$SiMe_2O$][1,2-$SiMe_2C_2B_{10}H_{11}$]}$_2C_2B_{10}H_{10}$ (FF)	S, H	[438]
1-{[$SiMe_2O]_2Si(CH_2)_3$}-7-Me	S, H	[438]
[$CB_{10}H_{10}C$-$SiMe_3]_2$ (FF)	S	[187]
{[($C_2B_{10}H_{11}$-1-C[O]O)(*n*-$C_4H_9)_2Si]_2O\}_2$ anti-tumor compound (FF)	X	[448]
—[—C≡C—C≡C—$SiMe_2$—O—$SiMe_2$—$CB_{10}H_{10}C$-$SiMe_2$-O-$SiMe_2$ —($CB_{10}H_{10}C$-$SiMe_2$—O—$SiMe_2)_z$—]— (*z* = 1, 3, 8) (FF) diacetylene-disiloxane polymers	S, H, C, IR, DSC, TGA (effect of concentration dilution of cross-linkable diacetylenes on plasticity)	[451]
—{$CB_{10}H_{10}C$—[($SiMe_2$—$O)_2$— $SiMe_2$—$CB_{10}H_{10}C]_x$— ($SiMe_2$-$O)_2$—$SiMe_2$-[C≡C—C≡C-($SiMe_2$-$O)_2$—$SiMe_2]_y\}_n$ (FF) diacetylene-disiloxane polymers	S, H(solid, var. temp.), C, IR, DSC, TGA (dependence of thermal properties on copolymer sequence)	[452]
—[Me_2Si-$CB_{10}H_{10}C(SiMe_2O]_m$—]$_n$ *m* = 1–3 (FF) siloxane copolymers	S, TGA, DTA	[453]
[—$CB_{10}H_{10}C$—($SiMe_2O)_2SiMe_2$—]$_n$ (FF) siloxy polymers	Ultrasound propagation; glass transition	[454]
{—Me_2Si—$CB_{10}H_{10}C[SiOMe_2]_m$—}$_n$ *m* = 3, 5 (FF) siloxy polymers, MW = 16,000–30,000 (soluble waxes and liquids)	S	[455]
{—Me_2Si-$CB_{10}H_{10}C[SiOMe_2]_2$-[$SiOMePh]_y(SiOMe_2)$—}$_n$ (*y* = 1, 2, 3) (FF) siloxy polymers	S	[455]
Exactly alternating carborane-siloxane polymers	S(stoichiometric polycondensation of cyclosilazanes with diols), TGA, STM	[828]
1,7-(—$SiMe_2$—O—$SiMe_2R)_2$ R = H. $CH{=}CH_2$, $CH_2CH{=}CH_2$	S, H, C, IR, MS	[831]
[—$SiMe_2$—O—$SiMe_2$—$CB_{10}H_{10}C$—$SiMe_2$—O—$SiMe_2$—C≡C—C_6H_4—*m*/*p*-C≡C—]$_n$ thermoset at 500 °C forms crosslinked siloxane-aryalacetylene polymer	S, C, Si, IR, TGA, DSC, XPS, dynamic mechanics analysis	[843]
1-CH_2SiMe_2Ph-7-R R = H, CH_2SiMe_2Ph	S, H	[894]
1-$CH_2SiMe_2(C_6H_4$-*p*-OMe)-7-R R = H, $CH_2SiMe_2(CC_6H_4$-*p*-OMe)	S, H, X(R = C_6H_4-*p*-OMe)	[894]
1,7-($CH_2SiMe_2X)_2$ X = Br, OH, H, $CH{=}CH_2$, C≡CH	S, H, X(OH)	[894]
Poly(dimethylsiloxane)-*co*-*m*-carborane hybrid elastomers; study of segmental dynamics	Broadband dielectric spectrometry	[863]
1,7-($SiMe_2$-O-$SiMe_2H)_2$ conversion to solvent-free liquid silicone resins	S, H, IR, DSC, TGA, dynamic mechanical analysis	[887]
B-$(CH_2)_n SiMe_2Cl$ *n* = 1, 2	IR (detailed study; inductive effect)	[460]
B-$(CH_2)_n SiMeCl_2$ *n* = 1, 2	IR (detailed study; inductive effect)	[460]

Compound	Information	References
B-CH_2SiCl_3	IR (detailed study; inductive effect)	[460]
B-$CH_2CH_2SiMe_3$	MS (detailed)	[461]
B,B′-$(CH_2CH_2SiMe_3]_2$	MS (detailed)	[461]
n-$CH_2CH_2SiCl_3$ *n*=1, B	MS (fragmentation patterns)	[715]
B-$CH_2CH_2SiR_3$ R=Cl, Me	S	[462]
B,B′-$(CH_2CH_2SiR_3)_2$ R=Cl, Me	S	[462]
B-$(CH_2)_2Si(OOR)_3$ R=CMe_3,CMe_2Et, 2-cyclohexylisopropyl peroxy	S	[258]
9-CH_2SiMe_3	S	[463]
Germanium		
1-$HgGeEt_3$-7-R R=H, Me, CH_2Cl, Ph	S	[465]
—[$GeMe_2$-$CB_{10}H_{10}C$—$SnMe)_2$-$CB_{10}H_{10}C]_n$ polymer (FF)	S	[466]
$HCB_{10}H_{10}C$-9-$HgGe(C_6F_5)_2Ge(C_6F_5)_2$-9-$CB_{10}H_{10}CH$ (FF)	S, IR	[467]
Tin		
1-$SnCl_2$	IR, Raman	[471]
$SnMe_3$-$CB_{10}H_{10}C$-7-Hg-$CB_{10}H_{10}C$-$SnMe_3$ (FF)	B (substituent effects), H, IR	[21]
1,7-$(SnR_3)_2$ R=*n*-C_4H_9, Ph	S	[472]
1,7-$[SnPh_2Cl]_2$	S	[472]
1-SnR_3-7-Ph R=Me, Ph	S	[474]
1-$SnEt_3$-7-R	^{119}Sn γ-resonance spectra; quadrupole splittings; acceptor properties of cage	[475]
1,7-$[SnMe_3]_2$-10-$(CH_2)_2SiMe_3$	X	[476]
1-[$(CH_2)_nC(O)O^-$ $SnMe_3^+$]-7-R *n*=0, 1; R=Me, Ph	Mössbauer, pK_a, E (half-neutralization potential)	[226]
1,7-[$(CH_2)_nC(O)O^-$ $SnMe_3^+]_2$ *n*=0, 1	Mössbauer, pK_a, E (half-neutralization potential)	[226]
1,7-$(SnR_3)_2$-B,B′-$[CH_2CH_2SiMe)_3]_2$ R=Me, Et	IR (detailed study; inductive effect)	[460]
1-SnMe)$_3$]-7-$SnEt_3$-B,B′-$[CH_2CH_2SiMe_3]_2$	IR (detailed study; inductive effect)	[460]
[-OC(O)-$CB_{10}H_{10}C$-C(O)O-Sn(OH)-]$_n$ (FF)	S, IR, molecular weight, COND, TGA, DTA	[477]
—[$GeMe_2$-$CB_{10}H_{10}C$—$SnMe)_2$-$CB_{10}H_{10}C]_n$ polymer (FF)	S	[466]
$(B\text{-}C_2B_{10}H_{11})_2SnMe_2$ (FF)	IR, Raman	[471]
2-$CH_2CH_2SnEt_3$	S	[478]
$C_2B_{10}H_{11}$-9-Sn{$CH[MeC(O)O]_2$}$_2$-Hg-Sn{$CH[MeC(O)O]_2$}$_2$-9-$C_2B_{10}H_{11}$ (FF)	S	[479]
9-$SnCl_2$[O,O′-3,6-$[CMe_3]_2$-*o*-simiquinolate]	S, H	[480]
9-$SnCl_3$-1,7-R_2 R=H, Me	S	[481]
$SnCl_2(9\text{-}R_2C_2B_{10}H_9)_2$ R=H, Me (FF)	S	[481]
Lead		
{[$(C_2B_{10}H_{11}$-1-C[O]O)(*n*-$C_4H_9)_2Pb]_2O\}_2$ anti-tumor compound (FF)	X	[448]
[—O(O)C$(CH_2)_m$-NH(O)C-$CB_{10}H_{10}C$-C(O)NH$(CH_2)_m$-C(O)O-Pb^{2+}—]$_n$ *m*=2, 6, 9 oligomeric salt (FF)	S	[402]

Continued

Compound	Information	References
Exo-Polyhedral Transition Metal Derivatives		
Chromium, molybdenum, and tungsten		
1-R-7-R′ R = $CH_2PhCr(CO)_3$, $PhCr(CO)_3$; R′ = H, Ph, CH_2Ph	MS (fragmentation study)	[499]
$Na_2[Mo_6I_8[OC(O)\text{-}C_2B_{10}H_{11}]_6$ hydrogel particles from β-cyclodextrin polymer and Mo clusters	S, UV(luminescence), H, B(2d), high transmission electron microscopy, laser flash photolysis	[878]
Manganese, technetium, and rhenium		
1-[*cyclo*-$(CO)_2(CF_3)M(CO)_4$]-7-Me M = Mn, Re)	S, ESR	[500]
1,9-*cyclo*-[N═NPh-$Re(CO)_4$]-7-Me	S	[501]
1,3-*cyclo*-[$(CH_2NMe_2Re(CO)_4$]-7-Ph	X	[502]
Iron		
1-CH_2(CO)Fe(CO)Cp-7-Me	S	[495]
1-CH_2(CO)Fe(CO)Cp-7-Me-9,10-Br_2	S	[495]
1-(η^6-naphthyl)$FeCp^+$	S, ESR	[510]
1-$CH_2C_5H_4$FeCp-7-Me	S, E	[511]
1-C≡CFe$(CO)_2$Cp	S	[512]
1-C(═CH_2)C_5H_4FeCp	S	[447]
Fe[C_5H_4-C(OH)Me$C_2B_{10}H_{11}]_2$ (FF)	S	[447]
9-$C_5H_4Fe(CO)_2Br$	S, H, B, IR	[514]
Cobalt		
9-CH_2-$C_2Co_2(CO)_6$	S	[169]
Co(phthalocyanine)(9-PhO-$C_2B_{10}H_{10})_4$ (FF)	S, IR, UV	[257]
Rhodium		
1-Rh[$PPh_3]_2$-7-R R = H, Me, Ph	S	[518]
{(C_8H_{12})Rh($C_{20}H_{12})_2$-O_2P-S—$C_2B_{10}H_{10}$}$^+$ BF_4^- chiral thiophosphite (FF)	S, H, B, P	[323]
Iridium		
1-Ir(H)[CH_2CH_2C(O)OR](CO)[PPh_3]-7-Ph [Ir-(O)] R = Me, Et	S, H, IR	[521]
1-{Ir(H)CH[C(O)OMe)CH_2C(O)OR](CO)[PPh_3]}-7-Ph [Ir-(O)] R = Me, Et	S, H, IR	[521]
1-{Ir(H)[CPh═CHC(O)OEt]—(CO)(PhCN)[PPh_3]}	S, H, IR	[521]
1-{Ir(H)C[C(O)OMe]═CHC(O)OMe(CO)-(RCN)[PPh_3]} R = Me, Ph	S, H, IR	[521]
1-{Ir(H)[C═CHC(O)OC(O)](CO)(PhCN)[PPh_3]}	S, H, IR	[521]
1-{Ir(H)(CO)(PhCN)[PPh_3][$CHCH_2$C(O)OC(O)]}	S, H, IR	[524]
($N_2C_{12}H_8$)Ir($N_2C_{10}H_8$—1,7 − $CB_{10}H_{10}CH)_2^+$ PF_6^- enhances phosphorescence emission	S, H, B, C, MS, UV, phosphorescence	[839]
(NC_5H_5-CN_4)Ir[NC_5H_5—*m*/*p*-C_6H_4—$C_2B_{10}H_9]^{n+}$ *n* = 0,1 (FF)	S, X, H, B, C, MS, E, UV, phosphorescence/luminescence	[880]
(SC_4H_2-C_5H_4N)Ir[($N_2C_{10}H_6$(CH═C—$CB_{10}H_{10}CH)_2]^+$ PF_6^- thienylpyridyl, 2,2′-bipyridyl	S, X, H, B, C, UV(absorption and emission), MS	[888]
Palladium and platinum		
1-{Pt[PEt_3][*cyclo*-$Et_2PCH_2CH_2$]}-7-R R = Me, Ph	S, H, P, IR`	[532]
[1,7-[*cis*-Cl$(NH_3)_2$Pt$(NH_2)(CH_2)_3]_2C_2B_{10}H_{10}]^{2+}$ (FF)	S, H, B, C, Pt	[535]

Compound	Information	References
[1,7-[*trans*-$Cl(NH_3)_2Pt(NH_2)(CH_2)_3]_2C_2B_{10}H_{10}]^{2+}$ $[OSO_2CF_3^-]_2$ (FF)	S, H, B, C, Pt, cytotoxicity studies	[535]
1,7-$[(CH_2)_3SPt(terpyridyl)]_2C_2B_{10}H_{10}^{2+}$ $[OSO_3CF_3^-]_2$ (FF)	S, H, B, C, Pt, MS, cell toxicity	[536]
9-$HgPt[PPh_3]_2Ge(C_6F_5)_3$-10-R R = H, $HgGe(C_6F_5)_3$	S, IR	[467]
$C_2B_{10}H_{11}$—9-Hg—$Pt[PPh_3]_2Ge(C_6F_5)_2Ge(C_6F_5)_2$— $Pt[PPh_3]_2$—Hg—9-$C_2B_{10}H_{11}$ (FF)	S, IR	[467]
Copper		
$[—O(O)C(CH_2)_m$-$NH(O)C$-$CB_{10}H_{10}C$-$C(O)NH(CH_2)_m$-$C(O)O$-$Cu^{2+}—]_n$ m = 2, 6, 9 oligomeric salt (FF)	S	[402]
Mercury		
1-$HgGeEt_3$-7-R R = H, Me, CH_2Cl, Ph	S	[465]
(*o*-phenanthroline)$_2Hg[C(O)O$-$CB_{10}H_{10}CH]_2$ (FF)	S	[545]
$MeCB_{10}H_{10}CHgCl$•*o*-phenanthroline (FF)	S	[546]
$(MeCB_{10}H_{10}C)_2Hg$•*o*-phenanthroline (FF)	S	[546]
1-R-9-HgX X = Cl, Br, I; R = H, Me, Ph	MS (detailed)	[547]
B-$[HgC(O)OCF_3]_n$ n = 1–3	S	[551]
B-HgR R = Et, I	S	[552]
9-HgCl•*o*-phenanthroline	S	[553]
9-$HgGe(C_6F_5)_3$	S, IR	[467]
9,10-$[HgGe(C_6F_5)_3]_2$	S, IR	[467]
$HCB_{10}H_{10}C$-9-$HgGe(C_6F_5)_2Ge(C_6F_5)_2$-9-$CB_{10}H_{10}CH$ (FF)	S, IR	[467]
9-$HgPt[PPh_3]_2Ge(C_6F_5)_3$-10-$HgGe(C_6F_5)_3$	S, IR	[467]
$HCB_{10}H_{10}C$-9-$HgGe(C_6F_5)_2Ge(C_6F_5)_2Pt[PPh_3]_2$-9-$CB_{10}H_{10}CH$ (FF)	S, IR	[467]
$Hg(C_2B_{10}H_9$-9,10-$Cl_2)_2$ (FF)	S, E (pK_a)	[555]
$Hg(C_2B_{10}H_{10}$-9-$R)_2$ R = H, Me (FF)	MS (detailed)	[547]
$R'Hg(RC_2B_{10}H_{11})$ R = Me, Ph; R′ = Me, Ph (FF)	S	[543]
$[1,7$-$PhC_2B_{10}H_{10}]Hg[1,2$-$PhC_2B_{10}H_{10}$ (FF)	S	[543]
$Hg\{9$-$[Me_3Si]_2C_2B_{10}H_9]\}_2$ (FF)	S	[558]
$HgS(9$-$C_2B_{10}H_{11})_2$ (FF)	S	[332]
$HgM(9$-$C_2B_{10}H_{11})_2$ M = Se, Te (FF)	S, MS	[490,491]
$(9$-$C_2B_{10}H_{11})Hg(10$-*nido*-7,8-$C_2B_9H_{10}$-7-$R)^-$ R = H, Ph, $CHMe_2$ (FF)	S, H, B	[559]
9-Me-10-HgR R = $CF_3C(O)O$, Cl	S, B	[496]
$C_2B_{10}H_{11}$-9-ClHg-$C_2B_{10}H_{10}$-10-Me (FF)	S, B	[496]
$C_2B_{10}H_{11}$-9-$CF_3C(O)OHg$-$C_2B_{10}H_{10}$-10-X X = Cl, Br, I, Me (FF)	S, B	[496]
$C_2B_{10}H_{11}$-9-$Sn\{CH[MeC(O)O]_2\}_2$-Hg-$Sn\{CH[MeC(O)O]_2\}_2$-9-$C_2B_{10}H_{11}$ (FF)	S	[479]
$[(t$-$C_4H_7)Me_2Si]_2C_2B_{10}H_8$-9,10-$(HgX)_2$ X = Cl, $OC(O)CF_3$ (FF)	S, H, B, C, Hg, MS	[560]
Other Experimental Studies		
1-Li	Reaction with 1,2,4-triazine 4-oxides; nucleophilic substitution of H to form 1,2,4-triazin-5-yl derivatives OR ring transformation of the 1,2,4-triazine ring into the triazoline ring	[569]

Continued

Compound	Information	References
Theoretical Studies		
Molecular and electronic structure calculations		
1-SH	Charge distribution	[309]
n-SH *n*=1, 4, 9	EHMO, NEMO; charge distribution	[176]
9-$SCH_2C(O)OH$	EHMO, NEMO; charge distribution	[176]
1-Cl	Dipole moment	[344]
9-X X=Cl, Br, I	Dipole moment	[363]
1-Br	Dipole moment	[344]
1,7-Br_2, 9,10-Br_2	Dipole moment	[68,363]
$H_2C_2B_{10}X_{10}$ X=Cl, Br (FF)	Dipole moment	[68,363]
9,10-I_2	Dipole moment	[363]
1-I	Dipole moment	[344]
$Hg(n\text{-}C_2B_{10}H_{11}\}_2$ *n*=1, 9 (FF)	Raman (vibrational frequencies)	[485]
$RHg[9\text{-}(1,2\text{-}C_2B_{10}H_{11})]$ R=Et, Cl, Br, $AsCl_2$, $SbCl_2$	Raman (vibrational frequencies)	[485]
$(cyclo\text{-}O_2C_3Hme_2)Ir(N_2C_{10}H_8—1,7\text{-}CB_{10}H_{10}CH)_2$	DFT, HOMO-LUMO levels	[839]
$(N_2C_{12}H_8)Ir(N_2C_{10}H_8—1,7-CB_{10}H_{10}CH)_2^+ PF_6^-$	DFT, HOMO-LUMO levels	[839]
NMR calculations		
Parent	C	[33]
	B (paramagnetic contribution)	[596,597]
	B-H coupling	[598]
1,7-$(OH)_2$	C	[170]
9,10-X_2 X=Cl, Br, I	^{11}B shifts	[597]
	B (paramagnetic contribution)	[597]
Reactivity calculations		
1-$C(O)OOCMe_2C{\equiv}CH$-7-R R=H, $CHMe_2$ peroxy alkynes	$\Delta H_{formation}$, $\Delta G_{formation}$	[246]
1-$[C(O)OOCMe_2C{\equiv}C\text{-}CMe_2OOCMe_3]$ peroxy alkyne	$\Delta H_{formation}$, $\Delta G_{formation}$	[246]

[a] *Substituents on the carborane cage. "FF" indicates that the full formula of the compound is given.*
[b] *S, synthesis; X, X-ray diffraction; H, ^1H NMR; B, ^{11}B NMR; C, ^{13}C NMR; F, ^{19}F NMR; P, ^{31}P NMR; Li, ^7Li NMR; Si, ^{29}Si NMR; Pt, ^{195}Pt NMR; Hg, ^{199}Hg NMR; 2d, two-dimensional (COSY) NMR; IR, infrared data; MS, mass spectroscopic data; UV, UV-visible data; E, electrochemical data; ESR, electron spin resonance data; MAG, magnetic susceptibility; COND, electrical conductivity; OR, optical rotation; NLO, nonlinear optical properties; DSC, differential scanning calorimetry; TGA, thermogravimetric analysis; BNCT, boron neutron capture therapy; XRD, wide-angle X-ray diffraction.*