Appendix C

Supplemental Data for Table 8-1. Selected $CB_{11}H_{12}^-$ Derivatives

Compound	Information[a]	References
Synthesis and Characterization		
Nontransition Metal Derivatives		
No substituents on boron		
$CB_{11}H_{12}^-$	E (water-based electrolytes)	[323]
	IR	[3,147–149]
	Raman	[148]
	Counterion in silaoxazolinium salts	[337]
$Li^+CB_{11}H_{12}^-$ halogen-free electrolyte for lithium-ion batteries		[327]
$Mg(tetraglyme)^{2+}[CB_{11}H_{12}^-]_2$ electrolyte for Mg batteries	S, E, charge-discharge properties	[345]
$MgPh^+CB_{11}H_{12}^-$ oxidatively stable Mg battery electrolyte	S, X, H, E	[355]
$(n\text{-}C_5H_{11})CB_{11}H_{11}^-$	S, H, B, C	[324]
$Cp^*Fe(\eta^5\text{-}RNC_8H_5\text{-}NC_5H_{10})^+$ $CB_{11}H_{12}^-$ R=C(O)C(CH_2Ph)PhF	X	[315]
$[(2,6\text{-}MeOCH_2)_2C_6H_3]SnCr(CO)_5^+$ $CB_{11}H_{12}^-$	S, X, H, C, Sn	[259]
1-$[(CHMe_2)OP]CB_{11}H_{11}^-$	S, X, H, B, C, P, MS	[294]
1-$[H(HO)OP]CB_{11}H_{11}^-$	S, X, H, B, C, P, MS	[294]
1,2-*cyclo*-$[(CH_2)_4CHS(p\text{-}C_6H_4Me)]CB_{11}H_{10}^-$	S, X, H, B, C	[295]
[*cyclo*-$N(CH_2Ph)(CH_2)_3N(CH_2Ph)\text{-}C_6H_4\text{-}N(CH_2Ph)(CH_2)_3(N(CH_2Ph)\text{-}C_6H_4]^{2+}$ $[HCB_{11}Me_{11}^-]_2$ paracyclophane radical cation	S, X, H(var. T), E, IR, UV	[300]
(Distearoyl lipid)$CB_{11}H_{11}^{2-}$ $2K^+$ incorporation in liposomes for BNCT	S, biodistribution in mice	[285]
$(Me_2CH)_2P\text{-}CB_{11}H_{11}^-$	S, X	[288]
$C_4H_4S\text{-}Au\text{-}P(Me_2CH)_2\text{-}CB_{11}H_{11}$ catalysis of hydroamination of alkynes with amines	S, X, H, P	[288]
$Porphyrin(p\text{-}C_6H_4\text{-}CB_{11}H_{11})_4^{4-}$ $4Cs^+$ amphiphilic polymers for photodynamic therapy		[278]

Continued

Compound	Information	References
Porphyrin$[C_6F_4$-*p*-$CB_{11}H_{11}]_4^{4-}$ $4Na^+$	S, COND, permeation of bilayer lipid membranes	[281]
(Porphyrin)$[C_6F_4$-S$(CB_{11}H_{11})]_4^{4-}$ for BNCT and PDT	S, H, B, F, IR, UV, MS, cytotoxicity against HCT116 cell line	[344]
M(porphyrin)$[C_6F_4$-S$(CB_{11}H_{11})]_4^{4-}$ M = Cu, Zn Pd for BNCT and PDT	S, H, B, F, IR, UV, MS, cytotoxicity against HCT116 cell line	[344]
$H_{11}B_{11}C$-*cyclo*-$N_2C_3H_3$-$CB_{11}H_{11}^-$ *N*-heterocyclic carbene	S, H, C, Li	[313]
$H_{11}B_{11}C$-*cyclo*-$N_2C_3H_2Li$-$CB_{11}H_{11}^{2-}$ (two isomers) *N*-heterocyclic carbenes	S, X, H, C, Li	[313]
$\{H_{11}B_{11}C$-*cyclo*-$N_2C_3HLi_2$-$CB_{11}H_{11}^-\}_2$ *N*-heterocyclic carbene	S, X, H, C, Li	[313]
Cyclo-[1,3-$(C_6H_2Me_3)$NCH=CHN$(CB_{11}H_{11})$CH=] *N*-heterocyclic carbene/y/H/C/Li	S, H, C, Li	[339]
Cyclo-[1,3-$(C_6H_2Me_3)$NHC=CHN$(CB_{11}H_{11})$C]$^-$ *N*-heterocyclic carbene	S, X, H, C, Li	[339]
Cyclo-[1,3-$(C_6H_2Me_3)$NC=CHN$(CB_{11}H_{11})$C]$^{2-}$ *N*-heterocyclic carbene	S, X, H, C, Li	[339]
$(MeOC_5H_4N)CB_{11}H_{11}$ pyridinium	S, X, H, B, C, MS, UV	[324]
1,2-*cyclo*-$[(MeC_6H_4SO_2)N_3]CB_{11}H_{10}$ azide	S, X, IR, MS	[299]
$Ph_2P(CH_2)_2$S-$CB_{11}H_{11}^-$	S, H, B, C, MS	[302]
Cis/*trans*-M$[Ph_2P(CH_2)_3$S-$CB_{11}H_{11}]^{2-}$ M = Pt, Pd	S, H, B, C, MS	[302]
NMe_4^+ $Rh[Ph_2P(CH_2)_3S-CB_{11}H_{11}]_2^-$	S, X, H, B, C, MS	[302]
$Rh[Ph=P(CH_2)_2S-9\text{-}1,7\text{-}C_2B_{10}H_{11}]_2^+$ $Rh[Ph_2P(CH_2)_3S-CB_{11}H_{11}]_2^-$	S, X, H, B, C, MS	[302]
1-$H_2NSO_2NHCH_2$-$CB_{11}H_{11}^-$	*In vitro* inhibition in carbonic anhydrase	[304]
Cs^+ $RCB_{11}H_{11}^-$ R=O$(CH_2)_4NMe_2(CH_2)_n$NH-*bicyclo*-$C_5HN_4(NH_2)$-*cyclo*-$C_4H_5(OH)(CH_2OH)$O *n* = 2,3 deoxyadenosines	S, H, B, C, cytotoxicity	[310]
Cs^+ $RCB_{11}H_{11}^-$ R=O$(CH_2)_2$-O$(CH_2)_2NMe_2(CH_2)_3$NH-*bicyclo*-$C_5HN_4(NH_2)$-*cyclo*-$C_4H_5(OH)(CH_2OH)$O deoxyadenosines	S, H, B, C, cytotoxicity	[310]
$RCB_{11}H_{11}^-$ R=C_6H_4-*m*-CN, C_6H_4-*m*-NO_2, $C_6H_3(CF_3)_2$, $C_{10}H_7$, C_6H_4-*o*-OMe, CH=CHPh, C≡CPh, C_4H_2SMe, C_4H_2S-C_4H_2S	S(Pd-catalyzed C-C cross-coupling), UV, mesogenic activity, androgen-receptor binding	[317]
$[H(O)CH^{15}N]CB_{11}H_{11}^-$	S, X, H, B, C, IR, Raman, MS	[322]
$(C^{15}N]CB_{11}H_{11}^-$	S, X, H, B, C, IR, Raman	[322]
C_6H_4-1,4-$(CB_{11}H_{11})_2^{2-}$	S(Pd-catalyzed C–C cross-coupling), UV, mesogenic activity, androgen-receptor binding	[317]
C_6H_3-1,3,5-$(CB_{11}H_{11})_3^{3-}$	S(Pd-catalyzed C–C cross-coupling), UV, mesogenic activity, androgen-receptor binding	[317]
1-$CH_2RCB_{11}H_{11}^-$ R = C_5H_{10}N-CH_2, $PhCH_2NHCH_2$, C_5H_5N	S, H, B. IR	[329]
$[2,6\text{-}(MeO)_2C_6H_3]SnPh_2^+$ $CB_{11}H_{12}^-$ stabilization by pincer-type triaryltin ligand	S, H, B, Sn, IR, MS	[150]
M⊂[2.2.2]cryptate$^+$ $CB_{11}H_{12}^-$ Ni(TMTAA)]$_3$ M = Na, K; Ni(TMTAA) = tetraazacyclotetradecinenickel(II)	S, X	[12]

Compound	Information	References
[*N*, *N*′-dialkylimidazolium]$^+$ $CB_{11}H_{12}^-$	S, X, H, IR	[90]
	S, X, UV, IR	[152]
$H_2C_2N_3R(HN_2)^+$ $CB_{11}H_{12}^-$ R = H, Me imidazolium, triazolium salts	S(aqueous), H, C, MS	[91]
Ph[2,6-$(MeOCH_2)_2C_6H_3$]Sn(μ-$CH_2)_2$Sn[2,6-$(MeOCH_2)_2C_6H_3$]Ph^{2+} $[CB_{11}H_{12}^-]_2$ catalyst for acetylation of alcohols	S, X, H, B, C, Sn, MS	[153]
(*p*-$BrC_6H_4)CB_{11}H_{11}^-$	S, H, B, C	[50]
$(H_3NCH_2)C_2B_{10}H_{11}^+$ $(MeCH_2)CB_{11}H_{11}^-$	S, X	[154]
$(Me_2C{=}NHCH_2)C_2B_{10}H_{11}^+$ $(MeCH_2)CB_{11}H_{11}^-$	S, X	[154]
$Ag^+(MeCH_2)CB_{11}H_{11}^-$	S, X	[154]
Li^+ $RCB_{11}H_{11}^-$ R = Et, *n*-C_3H_7, *n*-C_4H_9, *n*-C_6H_{13}, 2-EtC_6H_{12}	S, H, C, B, IR, MS	
$(Me_3N)CB_{11}H_{11}$	H, B, MS	[5]
	S, H, B, IR	[23]
	X	[157]
$(Me_2HN)CB_{11}H_{11}$	H, B, MS	[5]
	S, H, B, IR	[23]
$(NH_2Me)CB_{11}H_{11}$	S, H, B, IR	[23]
$(Me_2N)CB_{11}H_{11}^-$	X	[158]
$(NHMe)CB_{11}H_{11}^-$	S, H, B, IR	[23]
(C_5H_{11}-$C_7H_8N)CB_{11}H_{11}^-$ C_5H_{11}-C_7H_8N = pentylquinuclidine	S, X, B, C, H, IR	[39]
$(NHMeEt)CB_{11}H_{11}$	S, H, B, IR	[23]
(*p*-MeO-$C_6H_4)_nN(C_6H_4-p-1-CB_{11}H_{11})_{3-n}^-$ *n* = 0–2 emission efficiency in nonfluorescent compounds	S, H, C, UV, E	[347]
$LCB_{11}H_{11}^-$ L = MeS, HS	S, H, B, IR	[15]
(succinylamido)$CB_{11}H_{11}{}^{131}I$ biodistribution in mice	S, H, B, MS	[159]
[*N*, *N*′-dialkylimidazolium]$^+$ $CB_{11}H_{12}^-$	S, X, H, IR	[90]
[*N*, *N*′-dialkylimidazolium]$^+$ $RCB_{11}H_{11}^-$ R = Me, Et, C_3H_7, *n*-C_4H_9) ionic liquids	S, X(Me, Et), H, IR	[90]
1,2-(*cyclo*-N_3PhMe+)$CB_{11}H_{10}^-$ triazole zwitterion	S, E, UV	[309]
1,2-(*cyclo*-N_3PhMe)$CB_{11}H_{10}^{\cdot-}$ triazole radical anion	S, X, ESR, E, UV	[309]
$EtMeN_2C_3MeH_2^+$ $CB_{11}H_{12}^-$ 1,2-Me_2-3-Et-imidazolium ionic liquid	S, H	[160]
RNC_5H_5+ $CB_{11}H_{12}^-$ R = *n*-butyl-, *n*-hexyl-, *n*-octyl *N*-alkylpyridinium salts ionic liquids	S, X(*n*-C_4H_9), H	[160]
RNC_5H_5+ R′$CB_{11}H_{11}^-$ R′ = Me, *n*-C_4H_9 *N*-alkyl pyridinium salts ionic liquids	S, H	[160]
C_5H_{11}-$NC_5H_5^+$ $CB_{11}H_{12}^-$ *N*-pentylpyridinium ionic liquid reaction medium in catalytic dehalogenation of aromatic halides	S, H, B, C, IR	[161]
[2,6-$(MeOCH_2)C_6H_3$]$SbCl^+$ $CB_{11}H_{12}^-$ organoantimony(III) O–C–O pincer ligand	S, X, H	[162]

Continued

Compound	Information	References
Na[2.2.2]cryptate(CTV)$^+$ $CB_{11}H_{12}^-$ CTV = cyclotriveratrylene) supramolecular	X	[124]
$M(CTV)_2(H_2O)_3(dmf)_2^+$ $CB_{11}H_{12}^-$ M = Na, Cs, Rb; CTV = cyclotriveratrylene	S, X	[163]
$K(CTV)(H_2O)(OH)(dmf)_2^+$ $CB_{11}H_{12}^-$ CTV = cyclotriveratrylene	S, X	[163]
$X(CH_2)_nCB_{11}H_{11}^-$ X = Cl, n = 3–7; X = Br	S, H, B, C, IR, MS	[31]
$(MeCHOHCH_2)CB_{11}H_{11}^-$	S, H, IR	[18]
$(NMe{=}X)CB_{11}H_{11}^-$ X = CHOH, CHO, C(OH)Ph, (O)Ph	S, H, B, IR	[23]
$(HOCR)CB_{11}H_{11}^-$ R = H, n-C_3H_7, MeCH = CH, Ph, C_4H_4O	S, H, IR	[18]
D or hydrocarbon substituents on boron		
$MeCB_{11}H_{11}^-$	S, H, B, C, MS, E	[29]
$RCB_{11}H$-2,3,4,5,6,7,8,9,10,11-Me_{10}^- R = H, Me	S, H, B, C, MS, E	[29]
$CB_{11}Me_{12}^-$, $HCB_{11}Me_{11}^-$, $HCB_{11}Me_{10}$-12-H^-, $HCB_{11}Me_{10}$-12-I^- isoflurane (ClF_3C_2H-O-CF_2H) as a nonpolar electrochemical solvent	E(isoflurane, SO_2, MeCN, CH_2Cl_2)	[290]
$CB_{11}Me_n(CD_3)_{12-n}^-$ n = 0–12 radicals 16 isomers	S, ESR	[279]
$(Me_2N)CB_{11}H_{10}$-2-$CH_2NH(CHMe_2)_2$	S, X, B, H	[49]
$(Me_2NH)CB_{11}H_{10}$-2-CH_2Cl	S, X, B(2d), H	[164]
$MeCB_{11}H_{10}$-12-Me	S, H, B, C, IR, MS	[33]
$PhCB_{11}H_{10}$-12-C≡$CSiMe_3^-$	S(microwave-assisted Pd-promoted cross-coupling), H, B, C, P	[272]
$HCB_{11}H_9$-n-C≡CH-12-X^- n = 4,7; X = Cl, Br	S(microwave-assisted Pd-promoted cross-coupling), H, B, C, P	[272]
$HCB_{11}H_{10}$-2-NH_2-12-R^- R = C≡C-Ph, C≡C-$SiEt_3$	S, X(C≡C-Ph), H, B(2d), C, MS, Raman	[305]
$HCB_{11}H_{10}$-2-NMe_3-12-C≡CH	S, X, H, B(2d), C, MS, Raman	[305]
$[HO(O)C]CB_{11}H_{10}$-12-C≡CH^-	S, X, H, B, C, IR, Raman, MS	[322]
$[H_2N(O)C]CB_{11}H_{10}$-12-C≡CH^-	S, X, H, B, C, IR, Raman, MS	[322]
$(NC)CB_{11}H_{10}$-12-C≡CH^-	S, X, H, B, C, IR, Raman, MS	[322]
$[H(O)CHN]CB_{11}H_{10}$-12-C≡CH^-	S, X, H, B, C, IR, Raman, MS	[322]
$(CN)CB_{11}H_{10}$-12-C≡CH^-	S, X, H, B, C, IR, Raman, MS	[322]
1-$RCB_{11}H_{10}$-12-C≡C-$(C_5H_4)FeCp^-$ R = H, H_2N, Me_3N^+	S, X(H, H_2N), H, B, C, IR, Raman, MS, UV, E	N[90]
$Me_3N_3P_3Cl_6^+$ $HCB_{11}Me_5Br_6^-$ phosphazene cation	S, X, H, P	[165]
$H[P_3C_3(CMe_3)]^+$ $HCB_{11}Me_5X_6^-$ X = Cl, Br stable salt of phosphabenzene cation	S, X, H, P	[166]
Me_2Si(*bicyclo*-$C_6H_2Me_2C_6H_3$)-$C_6H_2Me_3^+$ $HCB_{11}Me_5Br_6^-$ silyl-stabilized allyl cation	S, X, H, C	[95]
$(Me_2N)CB_{11}H_{10}$-7-CH_2Ph	S, H, B(2d), MS	[32]
$(Me_3N)CB_{11}H_9$-2-Ph-8-X X = I, $CH_2{=}CHCH_2$	S, B(2d[I]), H*	[43]
1,2-[*cyclo*-$(CH_2)_3CHOR]CB_{11}H_{10}^-$ (two isomers) R = Me, Et	S, X(Et), H, B, C, IR	[283]
1,2-[*cyclo*-$(CH_2)_3CHR^+$ $CB_{11}H_{10}^-$ R = PPh_3, NH_2CMe_3, $NHEt_2$, S(*p*-C_6H_4Me), NEt_3 (two isomers), $C_{10}H_5N_2H_5^+$ (proton sponge), py (two isomers), *p*-NC_4H_4Me	S, X(NH_2CMe_3, $NHEt_2$, NEt_3, proton sponge, pyridine, *p*-NC_4H_4Me), H, B, C, IR	[283]

Compound	Information	References
1,2-[*cyclo*-$(CH_2)_3CH{=}CH]CB_{11}H_{10}^-$	S, X, H, B, C, IR	[283]
$PhCB_{11}H_{10}$-12-Ph^-	S, X, H, B, C	[40]
1-$CB_{11}H_{10}$-12-Ph^- Me_3NH^+	E (water-based electrolytes)	[323]
$(MeC_6H_4\text{-}C_6H_4)CB_{11}H_{10}$-12-$C_6H_4Me$	S, X	[38]
$(C_6H_{12}O_2)CB_{11}Me_{10}$-12-*p*-$C_6H_4Br^-$	S, X, H, B, C	[41]
$PtMe[P(CHMe_2)_3]_2^+$ $HCB_{11}Me_{11}^-$	S, X, H, B, C, MS	[130]
$Rh_6(Pcy_3)H_{16}^+$ $HCB_{11}Me_{11}^-$	X	[167]
$X(CH_2)_nCB_{11}Me_{11}^-$ X = Cl, Br; n = 3,4,7	S, H, B, C, IR, MS	[31]
Me_2BzN^+ $(CH_2)_nCB_{11}Me_{11}^-$	S, H, B, C, IR, MS	[31]
$(CH_2{=}CH)(CH_2)_{n-2}CB_{11}Me_{11}^-$	S, H, B, C, IR, MS	[31]
Polymers from $[CH_2{=}CH(CH_2)_{n-2}]CB_{11}Me_{11}^-$ Li^+	S, H, B, C, IR	[20]
$[MeC(O)O]CB_{11}Me_{11}^-$	S, H, B, C, IR, MS	[31]
$Rh(H)_2(H_2)(PR_3)_2^+$ $HCB_{11}Me_{11}^-$	S, X	[168]
$CB_{11}Me_{12}^{\bullet}$ stable radical	Dopant in electron-delocalized *p*-doped hexaarylbenzene cation-radical salts	[140]
1-$RCB_{11}Me_{11}$ R = Me_3N, $H_2C{=}CH$, $Me_2N(CH_2)_2$	S, H, B, C, IR, MS	[141]
1-$RCB_{11}Me_{11}$ R = $BrHC{=}CH$, $Me_3SiC{\equiv}C$	S, H, B, C, IR, MS	[141]
$^{\bullet}Me_{11}B_{11}C\text{-}CH{=}CH\text{-}CB_{11}Me_{11}^{\bullet}$ stable biradical	S, IR, MS	[141]
$^{\bullet}Me_{11}B_{11}C\text{-}C{\equiv}C\text{-}CB_{11}Me_{11}^{\bullet}$ stable biradical	S, IR, MS	[141]
o-(phenothiazinyl)$_2C_6H_4^+$ $CB_{11}Me_{12}^-$	S, X, H, C	[139]
Li^+ $CB_{11}Me_{12}^-$	Catalyst for pericyclic rearrangements	[136]
$HCB_{11}Me_9$-7,12-Cl_2^- $ZrCp^*_2(OH)_2^+$	S, X, H, B, MS	[117]
$[HCB_{11}Me_{10}$-12-$Cl^-]_2$ $\{Pt[CHMe_2)_3P]_2(\mu\text{-}Cl)^+\}_2$	S, X, H, B, MS	[117]
$HCB_{11}Me_{10}$-12-$C_6H_4F^-$ $HCB_{11}Me_{11}^-$ $(PPh_3)_2HIr^{2+}$	S, X, H, B, MS	[117]
CMe_3^+ $HCB_{11}R_5X_6^-$ R = H, Me; X = Cl, Br stabilization in condensed phases via hyperconjugation and H-bonding	S, H, IR	[346]
$CB_{11}H_{10}$-7-R-12-X^- R = C≡CPh, X = F, Cl, Br; R = C≡CSiMe$_3$, X = F	S, H, B, C, IR, Raman, MS	[35]
$[HO(O)C]CB_{11}H_{10}$-12-*n*-$C_6H_{13}^-$	pK_a, B, H	[276]
$CB_{11}H_{12}^-$ methylation with $CD_3OTf \rightarrow CB_{11}(CD_3)_x(CD_2H)_9H_z^-$ substitution products; H-D scrambling	S. H, B(2d), C	[298]
1-$[C(O)OC_6H_4$-*p*-$R]CB_{11}H_{11}$-12-C_6H_{13} R = $(CH_2)_2$-*bicyclo*-C_8H_{12}-*p*-C_5H_{13}, N = N-C_6H_4-*p*-OC_6H_{13}, OC(O)C_8H_{17} comparison with ionic analogues; effect of coulombic interactions on mesophase stability (FF)	thermal analysis, X-ray diffraction patterns	[326]
Si-containing substituents on boron		
$[HO(O)C]CB_{11}H_{10}$-12-C≡$CSiEt_3^-$	S, H, B, C, IR, Raman, MS	[322]
$(NC)CB_{11}H_{10}$-12-C≡$CSiEt_3^-$	S, H, B, C, IR, Raman, MS	[322]
$[H(O)CHN]CB_{11}H_{10}$-12-C≡$CSiEt_3^-$	S, H, B, C, IR, Raman, MS	[322]
$[HO(O)C]CB_{11}H_{10}$-12-C≡$CSiEt_3^-$	S, H, B, C, IR, Raman, MS	[322]

Continued

Compound	Information	References
N- or P-containing substituents on boron		
$CB_{11}H_{11}$-*n*-NMe_3 *n* = 2,12	S, H, B(2d) MS	[32]
$(NC_5H_4\text{-}CH_2)CB_{11}H_{10}$ N-B	S, X, H, B, MS	[9]
1-$RCB_{11}H_{10}^-$-12-R′ R = H, C_5H_{11} R′ = NC_5H_4-*p*-OMe^+, CN, $SCHNMe_2^+$	S, H, B, C, MS	[343]
1,2-(*cyclo*-N_3R)$CB_{11}Cl_{10}^-$ R = Ph, *p*-C_6H_4F, *o*/*p*-C_6H_4OMe, $C_6H_2Me_3$, *n*-C_4H_9, adamantyl	S, X(Ph), H, B, C, MS	[289]
1-$HCB_{11}H_{10}^-$-12-$CNMe_2^+$ ylide	S, X, H, B, C, MS, IR	[331]
1-$HCB_{11}H_{10}^-$-12-C(NHMe)=NH_2^+ ylide	S, X, H, B, C, MS, IR	[331]
$RCB_{11}H_{10}$-12-NC_5H_4-OC_7H_{15} R = H, *n*-C_5H_{11} pyridinium	S, H, B, C, MS, UV	[324]
$RCB_{11}H_{10}$-12-NC_5H_4-OMe R = H, *n*-C_5H_{11} pyridinium	S, X(H), H, B, C, MS, UV	[324]
$RCB_{11}H_{10}$-12-NH_2^- R = H, *n*-C_5H_{11}	S, H, B, C	[324]
(*n*-C_5H_{11})$CB_{11}H_{10}$-12-N≡C-CD_3	S, B, MS	[324]
$RCB_{11}H_{10}$-12-NC_4H_4(=O) R = H, *n*-C_5H_{11} pyridone	S, H, B, C	[324]
O- or S-containing substituents on boron		
$CB_{11}H_{11}$-12-OH^- Me_3NH^+	E (water-based electrolytes)	[323]
$CB_{11}H_{10}$-7,12-$(OH)_2^-$ Me_3NH^+	E (water-based electrolytes)	[323]
$CB_{11}H_{10}$-7,12-$[C(O)OH]_2^-$	S, X, B, pK_a	[333]
$CB_{11}H_{11}$-12-$O(CH_2)_2O^+$ dioxane zwitterion	S, X, H, B, IR, MS	[170]
$CB_{11}H_{10}$-μ(1,2)-$(CH_2)_3CHOMe^-$ R = OMe^-, PPh_3	S, X, H, B, C, IR	[171]
$MeCB_{11}H_{10}$-2-CH(OMe)Me^-	S, X, H, B, C, IR	[171]
$RCB_{11}H_{10}^-$-12-R′ R = H, C_5H_{11} R′ = $SC_5H_{10}^+$, $SCHNMe_2^+$	S, H, B, C, MS	[342]
$HCB_{11}H_{10}(OTf)^-$	S, H, B, F	[350]
$HCB_{11}Cl_{10}(OTf)^-$	S, X, H, B, F	[350]
$HCB_{11}H_8(OTf)_3^-$	S, X, H, B, F	[350]
$HCB_{11}H_5Br_5(OTf)^-$	S, X, H, B, F	[350]
F-, Cl-, Br-, or I-containing substituents on boron		
$CB_{11}H_{11}$-*n*-$C_6F_5^-$ *n* = 7,12	S, H, B	[14]
1-$(H_2N)CB_{11}F_{10}$-6-H^-	S, B, C, F	[144]
1-$HCB_{11}F_{10}$-*n*-NH_3 *n* = 2, 7, 12	S, X, H, B(2d), C, F(2d), IR (*n* = 12), pK_a	[354]
1-$HCB_{11}F_{10}$-*n*-NH_2^- = 2, 7, 12	S, X(*n* = 12), H, B(2d), C, F(2d), Raman (*n* = 12), MS, pK_a	[354]
$Cu(CO)_2^+$ $EtCB_{11}F_{11}^-$	S, X, IR	[120]
$Cu(CO)_4^+$ $(PhCH_2)CB_{11}F_{11}^-$	S, X, IR	[120]
1-$(Cl_2P)CB_{11}X_{11}^-$ X = H, F, Cl, Br, I	S, H, B, C, P, F, MS	[294]
Ph_4P^+ Me_2SiCl-CH_2-$CB_{11}Cl_{11}^-$	S, H, C, Si	[307]
Cs^+ $HCB_{11}Cl_{11}^-$ reagent for gas phase removal of alkali metal cations from peptide ions in presence of excess protons, in electrospray ionization mass spectrometry (ESI)	MS	[335]
$RCB_{11}Cl_{11}^-$ R = H, *n*-C_4H_9 anion for cycloaddition and C–H activation reactions of Ta alkylidynes		[336]

Compound	Information	References
H^+ $HCB_{11}Cl_{11}^-$ protonation of $EtCl \rightarrow Et^+$ $HCB_{11}Cl_{11}^- + HCl \rightarrow Et_2Cl^+$ $HCB_{11}Cl_{11}^- \rightarrow Bu^+$ $HCB_{11}Cl_{11}^-$	IR	[262]
$R_1R_2R_3C_9H_{12}^+$ $CB_{11}H_{11}^-$ $R_1 = R_2 = H$, $R_3 = n\text{-}C_3H_7$ oxatriquinones $R_3O^+ \ldots H^+$ bond	S, IR	[271]
$C_{12}H_{34}O^{2+}$ $[CB_{11}H_{11}^-]_2$ oxonium $R_3O^+ \ldots H^+$ bond	S, X, IR	[271]
$CB_{11}H_{10}$-7-NH_3-12-X X = F, Cl	S,H, B, C, MS	[287]
$[MeCB_{11}F_{11}^-]_2$ $[AlMe_2^+]_2$	S, X, H, F	[286]
$[2,6\text{-}(2,6\text{-}Cl_2C_6H_3)_2C_6H_3](H_2NCMe_3)_2AlEt^+$ $HCB_{11}I_6H_5^-$	S, X, H, B, C	[258]
$HCB_{11}H_5Cl_6^-$ counterion for R_3Si^+ in protein-catalyzed silyl-mediated coupling of fluoroarenes		[263]
$Me_2SiC_6H_3$-2,6-$(C_6H_2Me_2X)_2^+$ $HCB_{11}H_5Cl_6^-$ X = F, Cl stable terphenylsilylium ions	S, X(Cl), H, C, F, Si	[266]
$(Me_3Si)_2NNCSiMe_3^+$ $HCB_{11}H_5Br_6^-$ catalyst for trimerization of bis-silylated diazomethane	S, X, H, B, C, Si, IR	[280]
$C_{10}H_6[(n\text{-}C_4H_9)_2GeE]_2(\mu\text{-}H)^+$ $HCB_{11}H_5Br_6^-$ E = Ge, Si naphthyl catalyst for hydrodefluorination of alkyl and benzyl fluorides		[312]
CMe_3^+ $HCB_{11}X_{11}^-$ X = F, Cl, Br stabilization in condensed phases via hyperconjugation and H-bonding	DFT: IR, structure	[346]
CMe_3^+ $HCB_{11}R_5X_6^-$ R = H, Me; X = Cl, Br stabilization in condensed phases via hyperconjugation and H-bonding	DFT: IR, structure	[346]
1-*cyclo*-$(thf)_2LiN_3(PPh_3)$-$CB_{11}H_{10}$-2-Cl phosphazide	S, P, X, IR, MS	[299]
(MeO)C(O)-C_6H_4-*p*-$CB_{11}H_5Br_6^-$	S(Pd-catalyzed C–C cross-coupling), UV, mesogenic activity, androgen-receptor binding	[317]
$RCB_{11}H_{10}$-12-I R = H, C_5H_{11}	S, H, B, C, MS	[343]
$CB_{11}H_{10}$-2-NH_2-12-I^-	S, X, H, B(2d), C	[305]
$Ag^+CB_{11}H_6Cl_6^-$ cocatalyst with carbene-stabilized L_3P^+ cations for conversion of biaryl-substituted arenes into polycyclic arenes		[334]
$(Ph_3P)_2H_2Ir^+$ $CB_{11}H_6Cl_6^-$ olefin hydrogenation catalyst	S, X, H, B, P	[118]
$PhNC_{12}H_2Br_6^+$ $CB_{11}H_6Cl_6^-$	S, UV, ESR	[84]
	Effects on Me_3PO ^{31}P NMR and adsorption on solid acid catalysts	[177]
	IR study of $H(H_2O)_n^+$ structure	[78]
H^+ $HCB_{11}Cl_{11}^-$ Cl–H–Cl bridged linear polymer	IR (gas and solid), X	[72]
H^+ $HCB_{11}H_5X_6^-$ X = Cl, Br, I	Acid strength	[71]
$(i\text{-}C_3H_7)_3Si(o\text{-}C_6H_4Cl_2)^+$ $HCB_{11}Cl_{11}^-$ silylium ion	S, X, Si	[92]
$Et_3Si\text{-}H\text{-}SiEt_3^+$ $HCB_{11}Cl_{11}^-$ silylium ion	S, X, Si	[92]
$Me_3Si\text{-}H\text{-}SiMe_3^+$ $HCB_{11}Cl_{11}^-$ silylium ion	S, X, Si, IR	[92]
cyclo-$H_6C_3(SiMe_2)_2C{=}CHCMe_3^+$ $HCB_{11}H_5Br_6^-$ vinyl cation	X	[178]
$MeCB_{11}Cl_{11}^-$	S, X, H, B, C, IR, MS	[56]
$RCB_{11}Cl_{11}^-$ R = H, Me	X	[58]

Continued

Compound	Information	References
$In(C_7H_8)_3^+$ $HCB_{11}Cl_{11}^-$	S, X, H, B, C	[349]
$In(C_6H_5Br)_{1.5}^+$ $HCB_{11}Cl_{11}^-$	S, X, H, B, C	[349]
Ph_3PH^+ $HCB_{11}Cl_{11}^-$	S, H, B, C, P	[349]
IPr-H^+ $HCB_{11}Cl_{11}^{2-}$ IPr = 1,3-bis(2,6-diisopropylphenyl) imidazol-2-ylidine	S, X, H, B, C	[349]
(IPr-H^+)$_2$ $CB_{11}Cl_{11}^{2-}$ IPr = 1,3-bis(2,6-diisopropylphenyl) imidazol-2-ylidine	S, X, H, B, C	[349]
$In(PhC{\equiv}CMes_2)^+$ $HCB_{11}Cl_{11}^-$	S, X, H, B, C, P	[349]
[*N*, *N*′-dialkylimidazolium]$^+$ $CB_{11}H_6X_6^-$ X = Cl, Br	S, X, H, IR	[90]
$Cp_2ZrCH(SiMe_3)_2^+$ $HCB_{11}Me_5Br_6^-$	S, X, H, B	[179]
B(subphthalocyanine)$^+$ $HCB_{11}Me_5Br_6^-$	S, X	[180]
R_3E^+ $CB_{11}H_6$-6,7,8,9,10-Br_6^- E = Ge, Sn, Pb	S, X, H, IR	[351]
$(Ph_3P)_2H_2Ir^+$ $CB_{11}H_6Br_6^-$ olefin hydrogenation catalyst	S, X, H, B, P	[118]
$Et_3Si(SO_2)^+$ $HCB_{11}Me_5Br_6^-$ silylium ion	S, X, Si	[92]
$RhP(C_5H_4)_2(C_5H_7)\{C_6H_3(CF_3)_2B[C_6H_3(CF_3)_2]_4\}^+$ $CB_{11}H_6Br_6^-$ kinetic vs. thermodynamic factors in anion coordination	S, X, H, F	[183]
$CB_{11}H(OH)_5Br_6^-$	S, X, IR	[75]
$(2,4\text{-}C_6H_3Br_2)_3NCB_{11}H_6Br_6^-$	S, UV, ESR, IR	[87]
$(N_3)CB_{11}Br_{11}^-$ azido	S, H, B, C, IR, MS	[325]
$(N_3)CB_{11}H_5Br_6^-$ azido	S, X, H, B, C, IR, MS	[325]
$RCB_{11}H_5Br_6^-$ R = $SiMe_3$, $Si(CHMe_2)_3$, C_3H_5, CH_2Ph, $P(CMe_3)_2$, C_6F_5, C_3F_5, C_6F_{11}, Merrifield peptide resin	S, H, P[$P(CMe_3)_2$], F(C_6F_5, C_3F_5, C_6F_{11}), MS	[185]
Phenoxonium$^+$ $CB_{11}H_6Br_6^-$ vitamin E model compound	S, X, C	[186]
$MeCB_{11}HBr_{10}^-$	S, X, H, B, C, IR, MS	[21]
$(C_5H_{11}\text{-}C_7H_8N)CB_{11}H_{10}$-12-$I^-$ C_5H_{11}-C_7H_8N = pentylquinuclidine	S, B, C, H, IR, X, MS	[39]
R_3Si^+ $CB_{11}H_6Br_6^-$ R_3 = Et_3, $(Me_2CH)_3$, $(CMe_3)_3$, $(CMe_3)_2Me$	S, X, B, Si, IR	[187]
$Tl(C_7H_8)_2^+$ $CB_{11}H_6Br_6^-$	X	[112]
$(Me_3C)_3Si(OH)_2^+$ $CB_{11}H_6Br_6^-$	S, X, H, B	[188]
$(Me_3N)CB_{11}H_{10}$-12-I	S, H, B	[43]
$HCB_{11}H_{10}$-*n*-I^- *n* = 7,12	S, H, B	[15]
	B(2d), C, MS	[189]
$HCB_{11}H_9$-7-I-12-X^- X = F, Cl, Br, OH	S, H, B, B(2d), C, MS	[189]
$MeCB_{11}H_5$-7,8,9,10,11,12-I_6^-	S, H, B, C, IR, MS	[33]
$(Ph_3P)_2H_2Ir^+$ $CB_{11}H_6I_6^-$	S, X, H, B, P	[118]
$(MePh_2P)_2H_2Ir^+$ $CB_{11}H_6I_6^-$	S, X, H, B, P	[118]
$Ir(CO)(Ph_3P)_2(HCB_{11}H_5Cl_6)$ complex of Vaska's compound	S, H, B, P	[190]
Ir(CO)(arene)$(PPh_3)^+$ $HCB_{11}H_5Cl_6^-$ arene = C_6H_6, MeC_5H_5 complex of Vaska's compound	S, X, H, B, P	[190]

Compound	Information	References
$Ir(CO)_2(PPh_3)_2^+$ $HCB_{11}H_5Br_6^-$ complex of Vaska's compound	S, X, H, B, P	[190]
$IrClPh(CO)(PPh_3)_2^+$ $HCB_{11}Cl_{11}^-$ complex of Vaska's compound	S, X, H, B, P	[190]
$(n\text{-}C_8H_{17})_3NH^+$ $HCB_{11}I_{11}^-$	IR ($\nu_{N\text{-}H}$ as a measure of acid strength)	[73]
$(p\text{-}FC_6H_4)_2CF^+$ $HCB_{11}I_{11}^-$	S, X, IR	[88]
$(p\text{-}FC_6H_4)MeCF^+$ $HCB_{11}I_{11}^-$	S, X, IR	[88]
$(H_3N)CB_{11}I_6H_5$	S, H, B, IR, MS	[55]
$H(benzophenone)_2^+$ $HCB_{11}H_5Cl_6^-$	S, X	[83]
$H(PhNO_2)_2^+/H(OEt_2)_2^+/H(THF)_2^+$ $HCB_{11}H_5Cl_6^-$	S, X	[83]
1-$RCB_{11}H_{10}^-$-12-IPh^+ R = H, C_5H_{11} reaction with nucleophiles to form carbonitrile, pyridinium, sulfonium, thiol, actoxy, and amino derivatives	S, H, B, C	[343]
Transition metal σ- and μ-complexes		
$HCB_{11}Cl_{11}{\cdot}Zn(CH_2CHCH_2CPh_2CH_2NH_2)_3$	S, X, H, B, C	[268]
$PhHg(1\text{-}CB_{11}F_{11})^-$ Lewis acidity	S, X(Hg), IR, DSC	[257]
$Hg(CB_{11}H_{10}\text{-}12\text{-}I)^{2-}$	S, X, H, B(2d), C, Si, Hg, IR, Raman, MS	[328]
$Hg(1\text{-}CB_{11}H_{10}\text{-}12\text{-}C{\equiv}CR)^{2-}$ R = H, $(C_5H_4)FeCp$, $Si(CHMe_2)_3$	S, X(H), H, B(2d), C, Si, Hg, IR, Raman, MS, UV[(C_5H_4)FeCp], IR, E[(C_5H_4)FeCp]	[328]
$CB_{11}H_{12}\text{-}8\text{-}(\mu\text{-}H)\text{-}FeCp(CO)_2$	S, IR, X, H	[192]
$CB_{11}H_{12}\text{-}8(\mu\text{-}H)\text{-}FeCp(CO)_2XAg$ X = Cl, Br, I	S, IR, H	[192]
	S, X, UV, IR	[152]
$Fe(H_2O)(TPP)^+$ $CB_{11}H_6Cl_6^-$	S, X, Mössbauer, MAG, H, IR	[195]
$Fe(OH)(TPP)_2^+$ $CB_{11}H_6Cl_6^-$	S, X, Mössbauer, MAG, H, IR	[195]
M[porphyrinPh_4]CHOH-$CB_{11}H_{11}^-$ Cs^+ M = Co, Cu, none	S, MS, IR, UV, H (no metal)	[197]
$[M(2,2'-bipyridine)_3^+$ $[CB_{11}H_{12}^-]_2$ M = Co, Ni	S, MAG, IR, UV, COND	[147]
$M(en)_3^{2+}$ $[CB_{11}H_{12}^-]_2$ M = Co, Ni	S, IR, MAG, UV	[200]
M[porphyrin-CH(OH)]$CB_{11}H_{12}^-$ M = Co, Cu, 2H	S, H, cytotoxicity	[360]
$Cu(CO)_2^+$ $EtCB_{11}F_{11}^-$	S, X, IR	[120]
$Cu(CO)_4^+$ $(PhCH_2)CB_{11}F_{11}^-$	S, X, IR	[120]
$(C_8H_{12})(MeCN)_2Ir^+$ $MeCB_{11}F_{11}^-$ less coordinating than BF_4^- toward Ir		[201]
M^+ 1-$MeCB_{11}F_{10}$-12-$SiPh_3^-$ M = Cs, Ag	S, X, H, B, C	[202]
$(C_5H_4Me)_2Zr(Me)\text{-}CB_{11}H_{12}$ B-H-Zr	S, X, H, B	[204]
$Cp^*_2Zr(Me)_2CB_{11}H_{12}$ 3 B-H-Zr	S, X, H, B	[204]
$Cp'Mo(CO)_3^+$ $CB_{11}H_{12}^-$ Cp′ = Cp*, Cp	S, X, H, B, IR	[205]
$CB_{11}H_{12}\text{-}12\text{-}MoCp(CO)_3$	S, X, H, IR	[206]
$[MoCp(CO)_3]_2(\mu\text{-}I)^+$ $HCB_{11}Me_{11}^-$	S, H, B, IR	[133]
$[CpMo(CO)_3I{\cdot}Ag(CB_{11}H_{12}]_2$	S, X, H, B, Ag, IR	[206]
$Rh(CO)_4^+$ $EtCB_{11}F_{11}^-$	S, X, supplemental experimental. data	[207]
$(\eta^4\text{-}C_8H_{12})Rh(THF)_2^+CB_{11}H_{12}^-$	S, X, B	[208]

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Compound	Information	References
(diene)L_2Rh^+ $CB_{11}H_{12}^-$	S, H, B, P	[209]
(norbornadiene)Rh$(PPh_3)^+CB_{11}H_{12}^-/CB_{11}H_6Br_6^-$	S, H, B, P	[210]
$(Ph_3P)_2Rh^+$ $CB_{11}H_{10}$-*n*-CH═CH_2^- *n*=7, 12	S, H, B, P	[106]
(norbornadiene)$(Ph_3P)_2Rh^+$ $CB_{11}H_{10}$-*n*-R^- R=CH═CH_2; *n*=7,12	S, X, H, B, P	[106]
$(Ph_3P)_2$Rh-$CB_{11}H_{11}$-*n*-CH═CH_2 *n*=7,12 Rh-||	S, H, B	[106], [107]
(norbornadiene)$(Ph_3P)_2Rh^+$ $CB_{11}H_6$-2,4,8,10,12-Et_5^-	S, X, H, B, P	[106]
$(Ph_3P)_2Rh^+$ $RCB_{11}H_{11}^-$ R=Me, $Si(CHMe_2)_3$	S, X[$Si(CHMe_2)_3$], H, B, P	[106]
$(Ph_3P)_2Rh^+$ $MeCB_{11}H_8Et_3^-$	S, X, H, B, P	[106]
$(Ph_3P)_2[\eta^2$-$C_2H_4)_3]Rh^+$ $CB_{11}H_6Br_6^-$	S, X, H, B, P	[106]
$(Ph_3P)_2$Rh-$CB_{11}H_{11}$-*n*-Et *n*=7,12 Rh-$(\mu$-H$)_2$	S, H, B	[107]
$(Ph_3P)_2$Rh-$CB_{11}H_7Et_5$ Rh-$(\mu$-H$)_2$	S, H, B	[107]
$(Ph_3P)_2$Rh-$MeCB_{11}H_8Et_3$	S, X, H, B, MS	[107]
$(Ph_3P)_2Rh(MeCN)_x^+$ $MeCB_{11}H_8Et_3^-$	S, H, B	[107]
$(\eta^4$-$C_6H_8)Rh(PPh_3)_2^+$ $CB_{11}H_6Br_6^-$ intermediate in catalytic. dehydrogenation of cyclohexane to benzene	S, X, H, C, P	[211]
$H(C_3H_7)_3^+$ $HCB_{11}H_8^-(\mu$-H$)_3RhH_2^+$ R=$CHMe_2$, C_6H_{11}, *cyclo*-C_5H_9; X=H, Br	S, X(C_6H_{11}), H, B, P	[182]
$(R_3P)_2Rh_2(HCB_{11}H_{11})_2$ R=$CHMe_2$, C_6H_{11}, *cyclo*-C_5H_9	S, X(C_6H_{11}, Br), H, B, P	[182]
[$(CHMe_2)$P]$(H_2C$═C-$CMe_3)Rh(HCB_{11}H_5Br_6)$	S, X, H, B, P	[182]
[(C_6H_{11})P]$_2$(L)Rh$(HCB_{11}H_5Br_6)$ L=C_6H_9, C_5H_7	S, X(C_5H_7), H, B, P	[182]
[Cp*Rh$(\mu$-2-Cl)$]_3(\mu$-3-Cl$)^{2+}$ $CB_{11}H_6Br_6^{2-}$	S, X	[212]
$Rh_2(PPh_3)_4H_2(\mu$-H$)(\mu$-Cl$)^+CB_{11}H_{12}^-$	S, H, B, P	[210]
$[(Ph_3P)(Ph_2P$-Ph)$Rh^+]_2$ $[CB_{11}H_6Br_6^-]_2$	S, X, H, B, P	[210]
$Rh_6\{CH(CH_3)_2]_3P\}_6H_{12}^{2+}$ $[CB_{11}Me)_{11}H^-]_2$	S, X, H, P	[213]
$Pd[Ph_2P(CH_2)_2PPh_2]^{2+}$ $[CB_{11}H_{11}Cl]_2$	S, X	[214]
$\{Pd[Ph_2P(CH_2)_2PPh_2](CB_{11}H_{12})\}^+$ $CB_{11}H_{12}^-$	S, X,H,P	[214]
$Ag[NC(CH_2)_2CN]_5[CB_{11}H_{12}]_4$	S, X, IR	[110]
$N[C_6H_3(OMe)P(CHMe_2)_2]_2PdCl^+$ $HCB_{11}Cl_{11}^-$ diarylamido pincer ligands	S, X, H, P, IR, E	[332]
$N[C_6H_3FP(CHMe_2)_2]_2NiCl^+$ $HCB_{11}Cl_{11}^-$ diarylamido pincer ligands	S, X, H, P, IR, E	[332]
$[(Me_2HC)_2$P-$C_6H_4]_2$Si-Pt-R^+ R′$CB_{11}H_{11}^-$ 2 Pt-P R=I, Otf, Me, Ph, Mes; R′=H, Et pincer complexes	S, X, H, Si, Pt	[348]
$(\eta^3$-$C_3H_7)Pd^+$-$P(CHMe_2)_2$-$CB_{11}Cl_{11}^-$ Pd-Cl catalyzes vinyl addition polymerization of norbornene	S, X, H, B, P	[342]
$Ag^+/(R_3P)Ag^+/(Ph_3P)(Et_2O)_2Ag^+/(Ph_3P)_2Ag^+$ $HCB_{11}Me_{11}^-$	S, X(close Ag-Me contacts), H, B(2d), IR	[116]
$Ag(bpy)^+$ 1-$PhCB_{11}H_5I_6^-\cdot$MeCN bpy=bipyridyl 1-D polymer chain	S, X, IR	[50]
$Ag_2(bppz)_3^{2+}$ $[1$-$(BrC_6H_4)CB_{11}H_{11}^-]_2\cdot$MeCN bppz=bis-2-pyridylpyrazine 1-D polymer chain	S, X, IR	[50]

Compound	Information	References
Ag^+ $CB_{11}H_6$-7,8,9,10,11,12-X_6^- X = Cl, I	S, B(2d)	[175]
$(PPh_3)Ag^+$ $CB_{11}H_6Br_6^-$ catalyst for hetero Diels-Alder reactions	S, X, H, B, P, IR	[108,125]
$(Ph_3P)_2Ag^+$ $CB_{11}H_6Br_6^-$	S, B, P, IR	[108]
$(Ph_3P)Ag^+$ $CB_{11}H_{12}^-$	S, H, B, P, IR	[125]
$[(Ph_3P)Ag^+CB_{11}H_{12}]_2^{2-}$	S, X, B, P, IR	[108]
Ph_3PAg^+ $HCB_{11}Me_{11}^-$ Ag-CH_3 interactions	S, X, H, B(2d), IR	[129]
$PhAg(CB_{11}H_{12})_2$	S, X	[109]
$(C_5H_5N)_2Ag^+$ $HCB_{11}Br_5I_6^-$	X	[215]
$\{[(MeCN)_4Ag\text{-}3][Ag(CB_{11}Br_5I_6)_2]\}_n$	S, X	[215]
$[CpMo(CO)_3I{\cdot}Ag(CB_{11}H_{12}]_2$	S, X, H, B, Ag, IR	[205]
$[Ag(IMes)_2{}^+]_2$ $Ag_2(closo-CB_{11}H_{12})_4{}^{2-}$ IMes = dimesitylimidazol-2-ylidene	S, X, H, B	[216]
$CB_{11}H_{12}$-Ag-IrCl(CO)$(PPh_3)_2$	S, IR, B, P	[192]
$CB_{11}H_6Br_6$-Ag-IrCl(CO)$(PPh_3)_2$	S, IR, B, P	[192]
IrCl(CO)$(Ph_3P)_2$.Ag$(CB_{11}H_{12})$	S, X, IR	[217]
$[CpMo(CO)_3IAg(CB_{11}Br_6H_6]_2$	S, X, H, B, Ag, IR	[205]
$\left[MoCp(CO)_3I^+\ Ag(CB_{11}H_{11}Br)\right]_2^-$	S, X, H, B	[133]
$\{[MoCp(CO)_3I]_3.Ag^+{}_2[HCB_{11}Me_{11}{}^-]_2$	S, X, H, B, IR	[133]
$[CpMo(CO)_3I{\cdot}Ag(CB_{11}H_{12}]_2$	S, X, H, B, Ag, IR	[206]
$CB_{11}H_{12}$-Ag-IrCl(CO)$(PPh_3)_2$	S, IR, B, P	[192]
$CB_{11}H_6Br_6$-Ag-IrCl(CO)$(PPh_3)_2$	S, IR, B, P	[192]
IrCl(CO)$(Ph_3P)_2$.Ag$(CB_{11}H_{12})$	S, X, IR	[217]
$(Ph_3P)_2IrH_2(\mu\text{-}Br)_2CB_{11}H_6Br_4$	S, X, H, B, P	[219]
$(Ph_3P)_2IrH_2(\eta^2\text{-}C_2H_4)_nCB_{11}H_6Br_6$ $n = 2,3$	S, X($n = 3$), H, B, P	[219]
(chlorin)M-$CB_{11}H_{11}^-$ Cs^+ M = Pd, Sn$(OH)_2$, Zn light-independent cytotoxicity/photodynamic tumor therapy	S, H, B, MS, IR, UV	[220]
(chlorin)$\{(CH_2)_2C(O)N[CH_2C(O)ONa]_2\}Me_4(CH{=}CH_2)(OH){=}CH{-}CH{=}NO{-}(CH_2)_3NHC(O)CH_2$-S-$CB_{11}H_{11}{}^{2-}$ for photodynamic therapy and BNCT	S, H, UV, MS, *in vivo* tumor uptake	[330]
(chlorin)$[CH_2C(O)ONa]_2\}Me_4(CH{=}CH_2)(OH){=}CH{-}CH{=}NO{-}(CH_2)_3N[C(O)CH_2$-S-$CB_{11}H_{11}]$-$[(CH_2)_3NHC(O)CH_2$-S-$(CB_{11}H_{11})]^{4-}$ for photodynamic therapy and BNCT	S, H, UV, MS, *in vivo* tumor uptake	[330]
PtLL′(PP)$CB_{11}H_{12}^-$ L = THF, L′ = Me, PP = $(CMe_3)_2P(CH_2)_3P(CMe_3)_2$	S, H, B, C, P, IR	[105]
$Pt(NCMe)_2(PP)^+$ $CB_{11}H_{12}^-$ PP = $(CMe_3)_2P(CH_2)_xP(CMe_3)_2$ ($x = 2,3$), $CH_2C_6H_4CH_2$	S, H, B, C, P, IR	[105]
$[L_2P(CH_2)_3PL_2]Pt\text{-}CB_{11}H_{12}]^+$ $CB_{11}H_{12}^-$ 2 Pt-H-B L = C_6H_{11}, CMe_3	S, P, C, H, B, IR	[105]
$[(CMe_3)_2P\text{-}Z\text{-}P(CMe_3)_2]Pt\text{-}CB_{11}H_{12}]^+$ $CB_{11}H_{12}^-$ 2 Pt-H-B Z = $(CH_2)_2$, $CH_2C_6H_4CH_2$)	S, X[$(CH_2)_2$], H, B, C, P, IR	[105]
$CB_{11}H_{10}\left(HgOCOCF_3\right)_2^-$	S, B, IR, Raman	[44]

Continued

Compound	Information	References
$(Me_3N)CB_{11}H_{10}$-12-$HgOCOCF_3$	S, B, IR, Raman	[44]
$CB_{11}H_{11}$-12-$HgOC(O)CF_3$	S, X, H, B(Br)	[14]
$[1,3\text{-}(Me_3Si)_2C_5H_3]_2Ln^+$ $CB_{11}H_6Br_6^-$ Ln = Sm, Er	S, IR	[119]
Other Experimental Studies		
Reactivity and kinetics		
$CB_{11}H_{12}^-$	Me methacrylate plasticizer-free polymer; cation exchanger; ion-sensitive electrode; Ca-sensitive membrane sensors	[16]
$[CH_2{=}CH(CH_2)_{n-2}]CB_{11}Me_{11}^-$ Li^+	Polymerization via radical mechanism	[20]
$(diene)_{L_2Rh}^+$ $CB_{11}H_{12}$	Reaction with $H_2 \rightarrow$ *exo-closo*-rhodacarboranes	[209]
Catalysis		
$(\eta^3\text{-}C_3H_7)Pd^+\text{-}P(CHMe_2)_2\text{-}CB_{11}Cl_{11}^-$ Pd-Cl	Catalyzes vinyl addition polymerization of norbornene	[342]
Other applications		
$CB_{11}H_{12}^-$	Gravimetric determination	[225]
$RCB_{11}H_{10}$-12-R'^- R = C_7H_6, C_5H_4; R′ = C_5H_4, C_7H_6	Hyperpolarizability; NLO	[227]
$BP^+CB_{11}H_{12}^-$	Ionic liquid for binap-mediated asymmetric catalysis of acetophenone by 3,1,2-$H(Ph_3P)Rh(C_2B_9H_{10})$-3-$CH_2{=}CHCH_2CH_2$-(μ-Rh)]	[229]
Theoretical Studies		
Molecular and electronic structure calculations		
$CB_{11}H_{12}^-$	DFT, cage substitution	[237,238]
$[H_{11}B_{11}C\text{-}C{\equiv}C\text{-}CB_{11}H_{11}]^{n-}$ n = 1, 2	DFT, *ab initio*	[239]
$H_{112}B_{11}C\text{-}R\text{-}CB_{11}H_{11}^{\bullet}$ biradicals R = C≡C, CH=CH, CH_2CH_2	DFT: electronic structures	[340]
cyclo-$(CB_{11}H_{10})_3(CH_2)_3^{3\bullet}$ radical	DFT: electronic structures	[341]
$(CB_{11}H_9)_4(CH_2)_4^{4\bullet}$ radical	DFT: electronic structures	[341]
$RCB_{11}H_nMe_{11-n}^-$ R = H, Me	Potential energy surfaces, oxidation potentials	[29]
$(NC)CB_{11}H_{11}^-$ X = H, F. Cl, Br, I	DFT, stability	[22]
$CB_{11}Me_{11}$	DFT	[31]
$(C_5H_4)CB_{11}H_{10}$-12-$C_7H_6^-$	β (first hyperpolarizability); NLO	[151]
$CB_{11}H_{11}$-12-C_7H_6	β (first hyperpolarizability); NLO	[151]
$RCB_{11}H_{10}$-12-R'^- R = C_7H_6, C_5H_4; R′ = C_5H_4, C_7H_6	MNDO	[227]
$RCB_{11}H_{10}$-12-R'^- R = H, C_7H_6; R′ = C_7H_6, H	MNDO	[227]
$Fe(TPP)(C_8H_{10})[Ag(CB_{11}H_6Br_6)_2]$ TPP = tetraphenylporphyrinate	DFT	[193]
$Fe(TPP)(C_8H_{10})[CB_{11}H_6X_6]$ L = C_6H_6, C_7H_8 X = Cl, Br	DFT	[193]
$Fe^{III}(TipsiPP)^+$ $CB_{11}H_6Br_6^-$ 4-coordinate porphyrin cation	S, X, H, UV	[243]
Ph_3PAg^+ $HCB_{11}Me_{11}^-$	Structure; energy minimization	[129]
Me_3NH^+ $HCB_{11}X_{11}^-$ X = Cl, Br, I	Natural population analysis charges	[228]
Me_3NH^+ $HCB_{11}H_5Br_6^-$	Natural population analysis charges	[228]

Compound	Information	References
Me_3N-$CB_{11}H_9$-2-Ph-8-X X = I, CH_2=$CHCH_2$	Heat of formation; charge distribution	[43]
$(Me_3N)CB_{11}H_{10}$-12-I	Heat of formation; charge distribution	[43]
$(Ph_3P)Ag^+$ $HCB_{11}Me_{11}^-$	DFT geometry	[116]
$CB_{11}H_{11}$-12-R^- R=C≡CPh, Cl	DFT geometry	[35]
$C_{12}H_{34}O^{2+}$ $[CB_{11}H_{11}^-]_2$ oxonium R_3O^+…H^+ bond	DFT	[271]
$(CB_{11}H_{12})^q$(s) s = spin	Isomer counting formulas	[273]
$CB_{11}H_{12}^-$ methylation with CD_3OTf → $CB_{11}(CD_3)_x(CD_2H)_9H_z^-$ substitution products; H-D scrambling	DFT, geometry of reaction intermediate	[298]
1,2,3-*cyclo*-(C_8H_{12})Ir$[P(CHMe_2)_2]^+$-1-$CB_{11}H_{11}^-$ 2 Ir-H-B agostic bonds	DFT, MOs	[301]
$HCB_{11}H_{10}$-2-NH_2-12-R^- R=C≡C-Ph, C≡C-$SiEt_3$	DFT, bond lengths, NMR	[305]
$HCB_{11}H_{10}$-2-NMe_3-12-C≡CH	DFT, bond lengths, NMR	[305]
Me_3N-$CB_{11}H_{10}$-12-C≡CH	DFT: bond lengths, NMR	[305]
$(p$-MeO-$C_6H_4)_nN(C_6H_4-p-1-CB_{11}H_{11})_{3-n}^-$ n=0–2	DFT: orbital energies	[347]
$RCB_{11}H_{11}^-$ R=C_6H_4-*m*-CN, C_6H_4-*m*-NO_2, $C_6H_3(CF_3)_2$, $C_{10}H_7$, C_6H_4-*o*-OMe, CH=CHPh, C≡CPh, C_4H_2SMe, C_4H_2S-C_4H_2S	DFT: energy levels	[317]
C_6H_4-1,4-$(CB_{11}H_{11})_2^{2-}$	DFT: energy levels	[317]
C_6H_3-1,3,5-$(CB_{11}H_{11})_3^{3-}$	DFT: energy levels	[317]
(MeO)C(O)-C_6H_4-*p*-$CB_{11}H_5Br_6^-$	DFT: energy levels	[317]
NMR calculations		
1-$(H_2N)CB_{11}F_{10}$-6-X^- X = H, OH	B, F	[144]
1-$(H_2N)CB_{11}F_9$-4,6-$(OH)_2^-$	B, F	[144]
Ag^+ $CB_{11}H_6$-7,8,9,10,11,12-X_6^- X = Cl, I	IGLO	[175]
$[HO(O)C]CB_{11}H_{10}$-12-C≡CR^- R = H, $SiEt_3$	DFT: electronic structure, NMR	[322]
$[H_2N(O)C]CB_{11}H_{10}$-12-C≡CH^-	DFT: electronic structure, NMR	[322]
$(^{15}NC]CB_{11}H_{11}^-$	DFT: electronic structure, NMR	[322]
$(NC)CB_{11}H_{10}$-12-C≡CR^- R = H, $SiEt_3$	DFT: electronic structure, NMR	[322]
$[H(O)CH^{15}N]CB_{11}H_{11}^-$	DFT: electronic structure, NMR	[322]
$[H(O)CHN]CB_{11}H_{10}$-12-C≡CR^- R = H, $SiEt_3$	DFT: electronic structure, NMR	[322]
$(C^{15}N]CB_{11}H_{11}^-$	DFT: electronic structure, NMR	[322]
$(CN)CB_{11}H_{10}$-12-C≡CH^-	DFT: electronic structure, NMR	[322]
Reactivity calculations		
$CB_{11}H_{12}^-$	*Ab initio*, electrophilic substitution	[246]
	Brønsted acidity	[62]
	DFT mechanism of formation from $B_{11}H_{14}$	[247]
$Li^+@CB_{11}H_{12}^-$	Photochemical release of endohedral Li^+	[248]
$HCB_{11}H_{10}$-12-C≡CH^-	DFT: structure	[36]
H^+ $CB_{11}H_{12}^-$	DFT: structure, gas phase Brønsted acidity	[74]

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Compound	Information	References
$H^+ CB_{11}X_nH_{12-n}^-$ X = Me, F, Cl, Br, I, CN, CF_3 n = 1, 6, 11, 12	DFT: structure, gas phase Brønsted acidity	[74]
$MeCB_{11}F_{11}^-$	DFT: MOs	[202]
$CB_{11}H_{11}Br^-$	*Ab initio*, electrophilic substitution	[246]
$HCB_{11}H_5X_6^-$ X = Br, Cl, F	Molecular electrostatic potential; acidity	[65]
$HCB_{11}Me_5Cl_6^-$	Molecular electrostatic potential; acidity	[65]
$HCB_{11}(CF_3)_nF_{11-n}^-$ n = 5, 6, 10, 11	DFT: electron detachment energy	[256]
1-HCB11Cl11-*n*-Ph n = 7,12	Transition state for silylium-F- $HCB_{11}Cl_{11}$ complex	[255]
Other calculations		
$RCB_{11}Me_{11}^-$	DFT: 2nd order NLO properties as a function of R substituent	[306]
1,2-(*cyclo*-N_3PhMe+)$CB_{11}H_{10}^-$ triazole zwitterion	DFT: molecular orbitals	[309]
$CB_{11}H_{12}^-$ and 1,12-$C_2B_{10}H_{12}$ isosteric pairs nematic liquid crystals	DFT: effect of molecular polarity on nematic phase stability	[316]
1-$RCB_{11}H_{10}$-12-C≡C-(C_5H_4)$FeCp^-$ R = H, H_2N, Me_3N^+	DFT, redox potentials	[338]
1-$ICB_{11}F_{11}^-$	Zero-point vibrational energy and B-X bond length (X = I, Xe) vs. 1-$XeCB_{11}F_{11}^+$ ions obtained via radioactive decay	[356]
1-$ClCB_{11}H_6$-2,3,4,5,6-Cl_5^-	Zero-point vibrational energy and B–X bond length (X = I, Xe) vs. $XeCB_{11}H_6Cl_5^+$ ions obtained via radioactive decay	[356]
1-$ClCB_{11}H_6$-7,8,9,10,11-Cl_5^-	Zero-point vibrational energy and B–X bond length (X = I, Xe) vs. $XeCB_{11}H_6$nnnnn ions obtained via radioactive decay	[356]

[a]S, synthesis; X, X-ray diffraction; H, ^{1}H NMR; B, ^{11}B NMR; C, ^{13}C NMR; F, ^{19}F NMR; P, ^{31}P NMR; Si, ^{29}Si NMR; Li, ^{7}Li 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; NQR, nuclear quadrupole resonance; DSC; differential scanning calorimetry.