Appendix G

Supplemental Data for Table 13-1. Selected 6- and 7-Vertex Transition Element Metallacarboranes

Synthesis and Characterization Yttrium 7-vertex closo-1,2,3-YC ₂ B ₄ clusters (C ₄ H ₈ O)(Cl)Y[(Me ₃ Si)RC ₂ B ₄ H ₄] ₂ Li(C ₄ H ₈ O) ₄ S, X(SiMe ₃), H, B. C, IR [8] (C ₄ H ₈ O) ₂ ClY[(Me ₃ Si) ₂ C ₂ B ₄ H ₄] ₂ ·OC ₄ H ₈ S, X, H, B, C, IR [10] {(Me ₂ C ₅ H ₅)Y[(Me ₃ Si)RC ₂ B ₄ H ₄] ₂ · OC ₄ H ₈ S, X, H, B, C, IR [11] Titanium [11] [11] 7-vertex closo-1,2,3-TiC ₂ B ₄ clusters [12] (n ⁸ -C ₈ H ₈)Ti(Et ₂ C ₂ B ₄ H ₃)-5-1 S, B, MS [12]	Compound ^a	Information ^b	References
Yttrium 7 -vertex closo-1,2,3-YC_2B_4 clusters $(C_4H_8O)(CI)Y[(Me_3Si)RC_2B_4H_4]_2Li(C_4H_8O)_4 R_3, N, B, C, IR [8] \{C_4H_8O)_2CIY[(Me_3Si)_2C_2B_4H_4]_2OC_4H_8 S, X, H, B, C, IR [10] \{(Me_2C_5H_5)Y[(Me_3Si)RC_2B_4H_4]\}_2 R=SiMe_3, M_6 S, X, H, B, C, IR [11] Titanium 7-vertex closo-1,2,3-TiC_2B_4 clusters S, B, MS [12] (\eta^8-C_6H_8)Ti(Et_2C_2B_4H_3)-5-1 S, B, MS [12] $	Synthesis and Characterization		
7-vertex closo-1,2,3-YC_2B_4 clusters $(C_4H_8O)(CI)Y[(Me_3Si)RC_2B_4H_4]_2Li(C_4H_8O)_4$ S, X(SiMe_3), H, B. C, IR [8] $\{C_4H_8O)_2CIY[(Me_3Si)_2C_2B_4H_4]_2.OC_4H_8$ S, X, H, B, C, IR [10] $\{(Me_2C_5H_5)Y[(Me_3Si)RC_2B_4H_4]_2.R=SiMe_3, Me^*$ S, X, H, B, C, IR [11] Titanium 7-vertex closo-1,2,3-TiC_2B_4 clusters [12] $(\eta^8-C_8H_8)Ti(Et_2C_2B_4H_3)-5-1$ S, B, MS [12]	Yttrium		
	7-vertex closo-1,2,3-YC ₂ B ₄ clusters		
$ \begin{cases} C_4H_8O)_2CIY[(Me_3Si)_2C_2B_4H_4]\}_2 \cdot OC_4H_8 & S, X, H, B, C, IR & [10] \\ \\ \{(Me_2C_5H_5)Y[(Me_3Si)RC_2B_4H_4]\}_2 R = SiMe_3, \\ Me & \\ \end{cases} S, X, H, B, C, IR & [11] \\ \hline \end{tabular}$	$(C_4H_8O)(CI)\mathbf{Y}[(Me_3Si)RC_2B_4H_4]_2Li(C_4H_8O)_4$ R=SiMe ₃ , Me	S, X(SiMe ₃), H, B. C, IR	[8]
$ \begin{cases} (Me_2C_5H_5)\mathbf{Y}[(Me_3Si)RC_2B_4H_4]\}_2 R = SiMe_3, \\ Me \end{cases} S, X, H, B, C, IR \qquad [11] \\ \hline \textbf{Titanium} \\ \hline \textbf{7-vertex closo-1,2,3-TiC_2B_4 clusters} \\ (\eta^8-C_8H_8)\mathbf{Ti}(Et_2C_2B_4H_3)-5-1 & S, B, MS & [12] \\ (n^8-C_8H_8)\mathbf{Ti}(Et_2C_2B_4H_3)-4.5-1_2 & S, B, MS & [12] \\ \end{cases} $	$\{C_4H_8O)_2CI\textbf{Y}[(Me_3Si)_2C_2B_4H_4]\}_2\cdot OC_4H_8$	S, X, H, B, C, IR	[10]
Titanium 7-vertex closo-1,2,3-TiC ₂ B ₄ clusters $(\eta^8-C_8H_8)$ Ti(Et ₂ C ₂ B ₄ H ₃)-5-1 S, B, MS [12] $(n^8-C_8H_8)$ Ti(Et ₂ C ₂ B ₄ H ₃)-4,5-12 S, B, MS [12]	$\label{eq:c2} \{(Me_2C_5H_5)\pmb{Y}[(Me_3Si)RC_2B_4H_4]\}_2 \ R\!=\!SiMe_3, \\ Me$	S, X, H, B, C, IR	[11]
7-vertex closo-1,2,3-TiC_2B_4 clusters $(\eta^8-C_8H_8)$ Ti(Et_2C_2B_4H_3)-5-1 S, B, MS [12] $(n^8-C_8H_8)$ Ti(Et_2C_2B_4H_3)-4.5-12 S, B, MS [12]	Titanium		
$(\eta^{8}-C_{8}H_{8})$ Ti $(Et_{2}C_{2}B_{4}H_{3})$ -5-1 S, B, MS [12] $(\eta^{8}-C_{8}H_{8})$ Ti $(Et_{2}C_{2}B_{4}H_{2})$ -4.5-1 S, B, MS [12]	7-vertex closo-1,2,3-Ti C_2B_4 clusters		
$(n^8-C_0H_0)\mathbf{Ti}(Et_3C_2B_4H_3)-4.5-I_2$ S. B. MS [12]	$(\eta^8 - C_8 H_8)$ Ti (Et ₂ C ₂ B ₄ H ₃)-5-1	S, B, MS	[12]
	$(\eta^8\text{-}C_8H_8)\textbf{Ti}(\text{Et}_2C_2B_4H_2)\text{-}4,5\text{-}I_2$	S, B, MS	[12]
$CpTi[R(Me_3Si)C_2B_4H_4]_2 R = SiMe_3, Me, H$ S, X(SiMe_3), ESR(SiMe_3), MAG, IR [14,15]	$\{CpTi[R(Me_{3}Si)C_{2}B_{4}H_{4}]\}_{2} R = SiMe_{3}, Me, H$	S, X(SiMe ₃), ESR(SiMe ₃), MAG, IR	[14,15]
$\{CpTi[Me(Me_3Si)C_2B_4H_4]\}_2$ S, X [16]	$\{Cp\textbf{Ti}[Me(Me_{3}Si)C_{2}B_{4}H_{4}]\}_{2}$	S, X	[16]
(Me_3P)_2Cl_2 Ti (Et_2C_2B_4H_4) ethyleneS, X, H, B, C, P, UV, IR[17]polymerization precatalyst	(Me ₃ P) ₂ Cl ₂ Ti (Et ₂ C ₂ B ₄ H ₄) ethylene polymerization precatalyst	S, X, H, B, C, P, UV, IR	[17]
$[Me_2P(CH_2)_nPMe_2]Me_2Ti(Et_2C_2B_4H_4) n=2,3 S, X, H, B, C, P, IR $ $[17]$ ethylene polymerization precatalysts	$[Me_2P(CH_2)_nPMe_2]Me_2Ti(Et_2C_2B_4H_4) n=2,3$ ethylene polymerization precatalysts	S, X, H, B, C, P, IR	[17]
$[O = P(NMe_2)_3](Me_3P)Cl_2Ti(Et_2C_2B_4H_4) $ S, H, C, P [17]	$[O = P(NMe_2)_3](Me_3P)Cl_2Ti(Et_2C_2B_4H_4)$	S, H, C, P	[17]
$\{[Me_2P(CH_2)_3PMe_2]MeTi(Et_2C_2B_4H_4)\}^+ S, H, C, P $ [17]	$\{[Me_2P(CH_2)_3PMe_2]Me\textbf{Ti}(Et_2C_2B_4H_4)\}^+$	S, H, C, P	[17]
$[Me_2P(CH_2)_3PMe_2][^{13}CH_3]_2Ti(Et_2C_2B_4H_4) S, H, B, C, P $ $[17]$ ethylene polymerization precatalyst	$\label{eq:me2} \begin{split} & [Me_2P(CH_2)_3PMe_2][{}^{13}CH_3]_2\mathbf{Ti}(Et_2C_2B_4H_4) \\ & \text{ethylene polymerization precatalyst} \end{split}$	S, H, B, C, P	[17]
Zirconium			
7-vertex closo-1,2,3-ZrC ₂ B ₄ clusters	7-vertex closo-1,2,3-ZrC ₂ B ₄ clusters		
$ \begin{bmatrix} (C_4H_8O)C \mathbf{Zr}[(Me_3Si)_2C_2B_4H_4]^{2-} \\ Li(C_4H_8O)_2^+ \end{bmatrix} S, X, H, B, C, IR $ [18]	$[(C_4H_8O)CI\textbf{Zr}[(Me_3Si)_2C_2B_4H_4]^{2-} \\ Li(C_4H_8O)_2^{+}$	S, X, H, B, C, IR	[18]

e154 APPENDIX | G Supplemental Data for Table 13-1. Selected 6- and 7-Vertex Transition Element Metallacarboranes

Compound	Information	References	
$\label{eq:masses} \begin{split} & [Mg(C_4H_8O)_3]_2(\mu\text{-CI})_3\text{Li-} \\ & [(Me_3Si)_2C_2B_4H_4]]_2 \textbf{Zr}(CH_2SiMe_3)\text{CI} \end{split}$	S, X, H, B, C, IR	[19]	
$LZrCI(OC_4H_8)(Et_2C_2B_4H_4) L = Cp, Cp^*$	S, H, B, C	[20]	
$(Me_3P)_2Cl_2\mathbf{Zr}(Et_2C_2B_4H_4)$ ethylene polymerization precatalyst	S, H, Р	[17]	
Hafnium			
7-vertex closo-1,2,3-HfC ₂ B ₄ clusters			
$Cl_2Cp^{\boldsymbol{*}}\boldsymbol{H}\boldsymbol{f}[Me(Me_3Si)C_2B_4H_4]_2\boldsymbol{\cdot}Li(OC_4H_8)$	S, H, B, C	[23]	
$Cl_3Cp^{\boldsymbol{*}}\boldsymbol{H}\boldsymbol{f}[(Me_3Si)_2C_2B_4H_4]_2\boldsymbol{\cdot}Li(OC_4H_8)$	S, H, B, C	[23]	
Niobium			
7-vertex closo-1,2,3-NbC ₂ B ₄ clusters			
$CpCl_2Nb(Et_2C_2B_4H_3-5-X) X = Cl, Br$	S, X(Br), H, B, C, MS	[25]	
Tantalum			
7-vertex closo-1,2,3-TaC ₂ B ₄ clusters			
CpLClTa($Et_2C_2B_4H_4$) L = Me, Et, CH ₂ Ph, CH ₂ CMe ₃	s, h, b, c, ir, uv, ms	[20]	
CpL_2 Ta ($Et_2C_2B_4H_4$) L = Me, Ph, CH2Ph, CH ₂ CMe ₃ , OPh	S, X(Ph), H, B, C, IR, UV, MS	[20]	
$\label{eq:cpl2} \begin{split} & CpL_2 \textbf{Ta}[(SiMe_3)_2 C_2 B_4 H_4 \ L = Me, \ CH_2 Ph, \\ & CH_2 CMe_3 \end{split}$	S, H, B, C, IR, UV, MS	[20]	
7-vertex closo-1,7,2,3-TaC ₂ B ₃ M clusters (triple-decker sandwiches)			
$Cp*Cl_2 \textbf{Ta}(Et_2C_2B_3H_3)\textbf{Co}Cp*$	S, H, B, C, IR, UV, MS	[20]	
$CpCl_2 \textbf{Ta}(Et_2C_2B_3Br_3)\textbf{Co}Cp^*$	S, X, H, B, C, MS	[25]	
$CpCI_2 \textbf{Ta}(Et_2C_2B_3HI_2) \textbf{Co}Cp^*$	S, H, B, MS	[20,25]	
Iron			
6-vertex nido-1,2,3-FeC ₂ B ₃ clusters			
<i>Nido</i> - $(\eta^6 - C_6 Me_6)$ Fe $(Et_2 C_2 B_3 H_{5-n} R_n) R_n = 5-$ Me, 4,5-Me ₂ , 4,5,6-Me ₃ , 5-CH ₂ Ph	S, H, B, IR, MS	[52]	
$\textit{Nido-}(\eta^{6}\text{-}C_{6}\text{Me}_{6})\textbf{Fe}(\text{Et}_{2}C_{2}B_{3}\text{H}_{3}\text{-}4\text{-}\text{I-}5\text{-}\text{Me})$	S, H, B, IR, MS	[52]	
$\textit{Nido-}(\eta^6\text{-}C_6\text{Me}_6)\textbf{Fe}(\text{Et}_2\text{C}_2\text{B}_3\text{H}_4)\text{-}5\text{-}\text{C}\textbf{=}\text{C}\text{H}$	S, H, B, C, IR, MS	[51]	
$\textit{Nido-}(\eta^5\text{-}Me_4C_4S)\textbf{Fe}(Et_2C_2B_3H_5) \text{ thiophene}$	S, H, B, IR, UV, MS	[55]	
$\begin{array}{l} 5\text{-}[\textit{nido-}(\text{Et}_2\text{C}_2\text{B}_3\text{H}_4)\textbf{Fe}(\text{PhCH}_2)]\text{-}\\ (\text{Et}_2\text{C}_2\text{B}_3\text{H}_4)\textbf{Fe}(\text{C}_6\text{Me}_6) \end{array}$	S, H, B, IR, MS	[57]	
p-[$nido$ -(C ₆ Me ₆) Fe (Et ₂ C ₂ B ₃ H ₄ -5- CH ₂)] ₂ (C ₆ H ₄) Fe (Et ₂ C ₂ B ₃ H ₄)	S, H, B, IR, MS	[57]	
Nido-(Et ₂ C ₂ B ₃ H ₄) Fe H(Et ₄ C ₄ B ₈ H ₇) B—B linked ligands	S, B, IR, MS	[58]	
7-vertex closo-1,2,3-FeC ₂ B ₄ clusters			
$H_2 \textbf{Fe}(Et_2 C_2 B_4 H_3 - 4 - Et)_2$	S, H, B, IR, MS	[72]	
$H_2 \textbf{Fe}[(Me_2 CH)_2 C_2 B_4 H_4]_2$	S, B, MS	[73]	
Cp_2Co^+ [Fe (Et_2C_2B_4H_4)_2]^-	S, H, UV, MAG	[75]	
$[CpFe(C_2B_4H_6)]^-$	S	[46]	
$Cp^{*}Fe(Et_{2}C_{2}B_{4}H_{4})$	Cytotoxic/antitumor activity	[34]	

Compound	Information	References
$Cp*Fe(Et_2C_2B_4H_3-5-X) X = Br, I$	S, H, IR, MS	[48]
$[(Et_2C_2B_4H_4)\textbf{Fe}H(C_5Me_4)]_2C_6H_4$	S, X, H, B, UV, E	[76]
$[(Et_2C_2B_4H_4)\textbf{Fe}(C_5Me_4)]_2C_6H_4$	S, H, B, UV, E, MAG	[76]
$\begin{array}{l} (\eta^6\text{-}C_6H_6) \textbf{Fe}(\text{Et}_2C_2B_4H_3)\text{-}5\text{-}(C_6H_5)\textbf{Fe}\text{-}\\ (\text{Et}_2C_2B_4H_4) \end{array}$	E	[78]
$[(\eta^6\text{-}C_6H_6)\textbf{Fe}(\text{Et}_2C_2B_4H_3)\text{-}5]_2$	E	[78]
$[(\eta^{6}-C_{6}H_{6})\mathbf{Fe}(Et_{2}C_{2}B_{4}H_{3})-5-]_{2}R R = C_{4}H_{2}S, C_{14}H_{10}, (C_{6}H_{4})_{n} n = 1,2$	E	[78]
$(\eta^6 - C_6 H_6)$ Fe (Et ₂ C ₂ B ₄ H ₃)-5-R X = H, I	Cytotoxic/antitumor activity	[34]
$(\eta^{6}-C_{6}H_{6})$ Fe (Et ₂ C ₂ B ₄ H ₃)-7-R R = Br, I, C=CSiMe ₃ , C=CH	S, H, B, C, IR, UV, MS	[51]
$(C_6H_6)\textbf{Fe}(Bu_2C_2B_4H_4)$	E	[81]
$[(\eta^6\text{-}C_6H_6)\textbf{Fe}(Et_2C_2B_4H_3)]_2CHMeCH_2$	S, X, H, B, IR, MS	[49]
$[(\eta^6\text{-}C_6H_5\text{-}C_6H_5)\textbf{Fe}(\text{Et}_2C_2B_4H_3)]_2$	S, H, IR, MS	[49]
$(\eta^6\text{-}C_6\text{H}_5\text{-}C_6\text{H}_5)\textbf{Fe}(\text{Et}_2\text{C}_2\text{B}_4\text{H}_4)$	S, X, H, C, B, IR, MS	[49]
	E	[79]
$\begin{array}{l} p \mbox{-}[nido\mbox{-}(\eta^{6}\mbox{-}C_{6}\mbox{Me}_{6})\mbox{Fe}(\mbox{Et}_{2}\mbox{C}_{2}\mbox{B}_{3}\mbox{H}_{4}\mbox{-}5\mbox{-} \\ C\mbox{H}_{2})]_{2}(\mbox{C}_{6}\mbox{H}_{4})\mbox{Fe}(\mbox{Et}_{2}\mbox{C}_{2}\mbox{B}_{4}\mbox{H}_{4}) \end{array}$	S, H, B, IR, MS	[57]
$(MeC_6H_5)\textbf{Fe}(Et_2C_2B_4H_4)$	S, X, H, B, C, IR, MS	[59]
$\begin{array}{l} p\mbox{-}[nido\mbox{-}(\eta^{6}\mbox{-}C_{6}H_{4}CHMe_{2})\textbf{Ru}(Et_{2}C_{2}B_{3}H_{4}\mbox{-}5\mbox{-}CH_{2})]_{2}(C_{6}H_{4})\mbox{-}\textbf{Fe}(Et_{2}C_{2}B_{3}H_{4}) \end{array}$	S, H, B, IR, MS	[57]
$(\eta^6\text{-}C_6\text{Me}_6)\textbf{Fe}(\text{Me}_2\text{C}_2\text{B}_4\text{H}_3\text{-}\text{C}_2\text{Me}_2\text{H}_3)$ (two isomers)	S, B, MS	[82]
$(\eta^6\text{-}C_8H_{10})\textbf{Fe}(\text{Et}_2C_2B_4H_3\text{-}\text{5-Br})$	S, H, B, C, MS	[48]
$(\eta^6 - C_8 H_{10})$ Fe [Ph(CH ₂) _n C ₂ B ₄ H ₅] n=2,3	S, H, B,IR, MS	[53]
$(\eta^{6}-C_{8}H_{10})Fe{[(CO)_{3}CrPhCH_{2}](PhCH_{2})-C_{2}B_{4}H_{4}}$	S, H, B, IR, MS	[83]
$(\eta^6\text{-}C_8H_{10})\textbf{Fe}\{[(CO)_3CrPhCH_2]_2C_2B_4H_4\}$	S, H, B, IR, MS	[83]
$[(\eta^{5}\text{-}C_{9}H_{7})H\textbf{Fe}(Et_{2}C_{2}B_{4}H_{4})]_{2}$	S, H, B, C, IR, MS, E	[54]
$(HNMe_2C_8H_4)\textbf{Fe}(Et_2C_2B_4H_4)$	Cytotoxic/antitumor activity	[34]
	E	[88]
$Fe\text{-wedged-}(C_4H_8O)_2\textbf{F}\textbf{e}_2(Et_2C_2B_4H_4)_2$	S, H, IR, UV	[89]
$B\text{-wedged-Cp}\textbf{FeCo}[(PhCH_2)_2C_2B_4H_4]_2$	S, H, B, IR, MS	[74]
$B\text{-wedged-}Cp\textbf{Fe}_2(Me_2C_2B_4H_4)_2$	B, IR	[91]
$(Me_2C_2B_4H_4) \textbf{Fe} H_2(Me_2C_2B_5H_5)$	S, H, B, IR, MS	[93]
$(Me_2C_2B_4H_4)\textbf{Fe}\textbf{H}_2(Me_2C_2B_7H_7)$	S, MS	[93]
<i>7-vertex closo-1,2,4-FeC₂B₄ clusters</i>		
$CpFe(C_2B_4H_5-C_{10}H_7)$	S, H, B	[46]
$Cp \textbf{Fe}(C_2B_4H_5\text{-}C_2B_5H_6)$	S, H, B, IR	[46]
7-vertex nido, closo-(2,3-C ₂ B ₃)Fe(2,3,5-C ₃ B ₂)M	carborane-diborolyl triple-decker sandw	iches)
$\label{eq:relation} \begin{array}{l} \textit{Nido, closo-}(Et_2C_2B_3H_5)\textbf{Fe}(Et_2MeC_3B_2Et_2)\textbf{-}\\ \textbf{CoCp} \end{array}$	S, MS	[98]

e156 APPENDIX | G Supplemental Data for Table 13-1. Selected 6- and 7-Vertex Transition Element Metallacarboranes

Compound	Information	References	
Nido, closo-[(PhCH ₂) ₂ C ₂ B ₃ H ₅] Fe -(Et ₂ MeC ₃ B ₂ Et ₂) Co Cp	S, MS	[98]	
$Cp \textbf{Fe}(Et_2 MeC_3 B_2 Et_2) \textbf{Fe} Cp$	E	[102]	
$Cp \textbf{Fe}(Me_2HC_3B_2Me_2)\textbf{Fe}Cp$	E	[102]	
$Cp \textbf{Fe}(Me_2HC_3B_2Me_2)\textbf{Co}Cp$	E	[102]	
$(CO)_3 \textbf{Fe} (MeEt_2C_3B_2Et_2) \textbf{Co}Cp$	S, IR, MS	[103]	
$(CO)_3 \textbf{Fe}(Et_2 MeC_3 B_2 Me_2) \textbf{Ni}Cp$	S, H, IR, MS	[103]	
$(CO)_3 \textbf{Fe}(Et_2 MeC_3 B_2 Me_2) \textbf{Ni}(CO)(\mu\text{-}CO)_2 FeCp$	S, H, B, IR, MS	[103]	
7-vertex closo, closo-(2,3- C_2B_4)Fe(2,3,5- C_3B_2)M	(carborane-diborolyl triple-decker sandw	viches)	
$[(PhCH_2)_2C_2B_4H_4]\textbf{Fe}(Et_2MeC_3B_2Et_2)\textbf{Co}Cp$	S, H, IR, UV, E, ESR, MS	[98]	
{[(PhCH ₂) ₂ C ₂ B ₄ H ₄] $Fe(Et_2MeC_3B_2Et_2)-CoCp$ } ^{<i>n</i>-} <i>n</i> =1,2	S, H, IR, E, ESR (n=2)	[98]	
Ruthenium			
6-vertex nido-1,2,3-RuC ₂ B ₃ clusters			
$[(MeC_6H_4-CHMe_2)Ru(Et_2C_2B_3H_3)]^{n-}$ n=1, 2	S	[96]	
$(MeC_6H_4CHMe_2)\mathbf{Ru}(Et_2C_2B_3H_4\text{-}5\text{-}CI)$	S, H, B, IR, MS	[114]	
6-vertex nido-1,2,4,5-Ru ₂ C ₂ B ₂ clusters			
$Cp*_2 \textbf{Ru}_2(Me_2C_2B_2H_5)\text{-}\mu\text{-}BH_2$	S, X, H, B, C, IR, MS	[115]	
$Cp*_2 Ru_2[HPhC_2B_2H_4Me]-\mu\text{-}BH_3$	S, H, B, IR, MS	[116]	
$Cp*_2 \textbf{Ru}_2[HPhC_2B_2H_3(CH_2CH_2Ph)]-\mu\text{-}BH_3$	S, X, H, B, IR, MS	[116]	
$Cp*_2\mathbf{Ru}_2[HPhC_2B_2H_6]-\mu$ -BH ₃	S, H, B, IR, MS	[116]	
$Cp*_2 Ru_2\{[MeC(O)]C_2B_2H_7\}$	S, X, H, B, C, IR, MS	[117]	
$Cp*_2 Ru_2 \{ [C(O)OMe] C_2 B_2 H_7 \}$	S, X, H, B, C, IR, MS	[118]	
$\begin{array}{l} Cp^{*}{}_{2}\textbf{R}\textbf{u}_{2}\{[C(O)OMe](BH_{2})C_{2}B_{2}H_{5}\}_{3}\text{-}(CH_{2})_{2}\text{-}\\ C(O)OMe \end{array}$	S, H, B, C, IR, MS	[118]	
$Cp*_2 Ru_2[(OMe)MeC_2B_2H_5-3-OH]$	S, X, H, B, C, IR, MS	[118]	
$Cp*_2 \textbf{Ru}_2 \{[B(OH)_2][C(O)OMe]C_2B_2H_6\}$	S, X, H, B, C, IR, MS	[118]	
$Cp^*{}_2H_2\textbf{Ru}_2(Me_2C_2B_2H_3)\text{-}3\text{-}CMeCMeB\text{-}(CMeCHMe)_2$	S, H, B, IR, MS	[119]	
$Cp^{*}{}_{2}H_{2}\textbf{Ru}_{2}(PhC_{2}B_{2}H_{5})\text{-}3\text{-}(CH_{2})_{2}Ph\text{-}\mu(BH_{2})$	S, H, B, IR, MS	[119]	
$Cp*_{2}H_{2}\textbf{Ru}_{2}[(Me)(MeO)C_{2}B_{2}H_{3}]\text{-}3\text{-}OH$	S, X, H, B, C	[120]	
6-vertex nido-1,2,3,5-RuC ₃ B ₂ clusters (diborolyl complexes)			
$Cp^{*}(CO)\textbf{Ru}(Et_{2}MeC_{3}B_{2}EtR) R = Et, CMe_{3}$	S, X(CMe ₃), H, B, C, MS	[62]	
$\label{eq:cp_star} \begin{split} &Cp^*(Me_3CNC) \textbf{Ru}(R_2R'C_3B_2R''_2) \ R, \ R', \\ &R''=Me, \ Et, \ Bu, \ CH_2SiMe_3 \end{split}$	S, X(Et, Et, Me; Et, Me, Me), H, B, C, MS	[122]	
$Cp^{*}H_{2}Ru(R_{2}R'C_{3}B_{2}R''_{2}) R, R', R'' = Me, Et, Bu, CH_{2}SiMe_{3}$	S, H, B, C, MS	[122]	
$Cp*{\it Ru}(PR_2R')(Me_3C_3B_2Me_2) \ R, \ R'=H, \ Ph, \\ Me$	S, H, B, C, MS	[123]	
$Cp^{*}\textbf{Ru}(Me_{3}C_{3}B_{2}Me_{2})_{2}(CS_{2})_{2}$	S, H, B, C, MS	[123]	
7-vertex closo-1,2,3-RuC ₂ B ₄ clusters			
$Cp^{*}H\textbf{Ru}(Et_{2}C_{2}B_{4}H_{3}\text{-}5\text{-}Me)$	S, H, B, C, MS, UV	[125]	

Compound	Information	References
$(MeC_6H_4\text{-}CHMe_2)\mathbf{Ru}(Et_2C_2B_4H_3\text{-}5\text{-}CI)$	S, H, C, MS	[114]
$L\textbf{Ru}(R_{2}C_{2}B_{4}H_{4}) L = 1,4\text{-}CHMe_{2}C_{6}H_{4}Me, \\ C_{6}H_{6}$	E	[81]
$(C_{10}H_{14}) \textbf{Ru}[(Me_{3}Si)_{2}C_{2}B_{4}H_{4}]$	S, H, B, IR, MS	[126]
7-vertex closo-1,2,4,5-Ru ₂ C ₂ B ₃ clusters		
$Cp_{2}^{*}Ru_{2}[HPhC_{2}B_{3}H_{4}]$ - <i>n</i> -(CH_{2}) ₂ Ph <i>n</i> =3,7	S, H, B, IR, MS	[116]
$Cp^{*}{}_{2}H_{2}\textbf{Ru}_{2}(PhC_{2}B_{3}H_{3})\text{-}3\text{-}(CH_{2})_{2}Ph$	S, H, B, IR, MS	[119]
7-vertex closo-1,7,2,3-RuC ₂ B ₃ M clusters (triple	-decker sandwiches)	
$\label{eq:closo_nido} \begin{split} & \textit{Closo, nido-}(\eta^6\text{-}MeC_6H_4CHMe_2)\mathbf{Ru-}\\ & (Et_2C_2B_3H_2Me)\text{-}\mathbf{Co}H(Et_2C_2B_3H_5) \end{split}$	S, H, B, UV, MS	[128]
$Cp^{*}\textbf{Ru}(Me_{3}C_{3}B_{2}Me_{2})\textbf{Rh}(Ph_{2}PCH_{2}CH_{2}PPh_{2})-Cl$	S, X, H, B, C	[134]
7-vertex 1,7,2,3,5-RuC ₃ B ₂ M (diborolyl triple-de	cker sandwiches)	
$Cp_{2}^{*}Ru_{2}(Me_{3}C_{3}B_{2}RCI) R = Me, CI$	S, X(Cl), H, B, MS	[1372]
$\begin{array}{l} (\eta^{6}\text{-}MeC_{6}H_{4}CHMe_{2})\textbf{Ru}(Et_{2}C_{2}B_{3}H_{2}R)\textbf{Os}(\eta^{6}\text{-}\\ MeC_{6}H_{4}CHMe_{2}) \ R \!=\! H, \ Cl) \end{array}$	S, H, B, IR, UV, MS	[96]
$Cp^{*}\textbf{Ru}(Me_{3}C_{3}B_{2}Me_{2})\textbf{Rh}(Et_{2}C_{2}B_{4}H_{4})$	S, H, B, C, MS	[136]
$Cp^{*}\textbf{Ru}(Me_{3}C_{3}B_{2}Me_{2})\textbf{Rh}(C_{2}B_{9}H_{11})$	S, H, B, MS	[136]
Cobalt		
6-vertex nido-1,2,3-CoC ₂ B ₃ clusters		
Cp Co (Me ₂ C ₂ B ₃ H ₄)- <i>nido</i> -Me ₂ C ₂ B ₄ H ₅ (two isomers)	s, h, b, ir, uv	[145]
$CpCo(Et_2C_2B_3H_3-4-X-6-Y) X = Br, Y = I;$ X=Br, Y=H; X=I, Y=H	S, H, B, C, IR, MS	[48]
$Cp^{*}Co(C_{2}B_{3}H_{6}Cl)$	S, H, B, IR, MS	[126]
$Cp^*Co(RC_2B_3H_6) R = CI, SiMe_3$	S, H, B, IR, MS	[126]
$Cp^{*}\textbf{Co}(Me_{2}C_{2}B_{3}H_{4})\text{-}5\text{-}Me$	S, H, B, IR, MS	[148]
$Cp*Co(Me_2C_2B_3H_3)-Me_2$ (two isomers)	S, H, IR, MS	[148]
$Cp^{*}Co(Me_{2}C_{2}B_{3}H_{4})-5\text{-}Cl$	S, H, IR, MS	[148]
$Cp^{*}Co(Me_{2}C_{2}B_{3}H_{4})-\mu-HgCl$	S, X, H, B, IR, MS	[150]
	B(2d)	[50]
$Cp^*Co(Et_2C_2B_3H_3)-4, 6-I_2$	Cytotoxic/antitumor activity	[34]
$Cp*Co(Et_2C_2B_3H_4)-5-R R = NMe_2, OCMe_3$	S, H, B, C, IR, MS	[152]
$R = C \equiv CH, C \equiv CSiMe_3$	S, H, B, C, IR, MS	[151]
$Cp^*Co(Et_2C_2B_3H_{5-n}R_n R_n = 4,5-Me_2, 4,5,6-Me_3$	S, H, B, IR, MS	[52]
$Cp^{*}Co(Et_{2}C_{2}B_{3}H_{4})$ -5- $OC_{4}H_{8}$	S, UV, MS	[154]
$Cp^{*}Co(Et_{2}C_{2}B_{3}H_{2})\text{-}Cl_{3}$	S, H, B, C, IR, UV	[154]
$Cp^{*}Co(Et_{2}C_{2}B_{3}H_{2})$ -5-Me-4,6-Cl ₂	S, H, B, C, IR, UV	[154]
$Cp*Co(RR'C_2B_3H_5) R = alkyl, arylalkyl$	S	[199]
$LCo(Et_2C_2B_3H_5)^{2-} L = Cp, Cp^*$	S	[96]

e158 APPENDIX | G Supplemental Data for Table 13-1. Selected 6- and 7-Vertex Transition Element Metallacarboranes

Compound	Information	References	
$(\eta^{5}\text{-}C_{5}Ph_{5})\textbf{Co}[(Me_{3}Si)_{2}C_{2}B_{3}H_{5}]$	S, H, IR, MS	[126]	
$(\eta^5\text{-}C_5H_4I)\textbf{Co}(Et_2C_2B_3H_5)$	S, H, B, C, IR, MS	[159]	
$[\eta^5\text{-}C_5H_4C(O)CI]\textbf{Co}(Et_2C_2B_3H_5)$	S, H, B, C, IR, MS	[160]	
$\label{eq:c2} \begin{split} &[(Et_2C_2B_3H_5)\textbf{Co}(\eta^5\text{-}C_5\text{Me}_4)C\text{=-}C]_2Pd\text{-}\\ &(Et_2NH)_2CI \end{split}$	S, MS	[161]	
$\begin{array}{l}({Et_2}{C_2}{B_3}{H_4}\text{-}5\text{-}C{H_2}{Ph})\textbf{Co}({C_5}{Me_4}\text{-}C{H_2}\text{-}\eta^5\text{-}\\{C_5}{H_4})\textbf{Fe}({Et_2}{C_2}{B_4}{H_4})\end{array}$	S, H, B, IR, MS	[86]	
$(\eta^{5}-PhCH_{2}C_{5}Me_{4})Co(Et_{2}C_{2}B_{3}H_{4}-5-R)R = H, CH_{2}Ph$	S, H, B, IR, MS	[86]	
$(\eta^{5}-NC_{4}Me_{2}R_{2})Co(Et_{2}C_{2}B_{3}H_{5}) R = Me, H$ pyrrolyl	S, H, B, IR, UV, MS	[129,162]	
$(B_9H_{12}-n-OC_4H_8)$ Co $(Et_2C_2B_3H_5)$ $n=5, 6$	S, H, B, IR, MS	[163]	
	X(n=5)	[164]	
Nido, closo- $(C_2B_3)Co(C_2B_4)$ complexes			
Closo, nido-($Et_2C_2B_4H_4$) Co H($Et_2C_2B_3H_4$ -5-n-C ₄ H ₉)	S, Н	[127]	
Nido, closo-(Me $_2C_2B_3H_5$)Co(Me $_2C_2B_4H_4$) ⁻	S, H, B, IR, MS	[165]	
$\begin{array}{l} Cp_2 \textbf{Co}^+ \; [\textit{nido, closo-}(Et_2 C_2 B_3 H_4 \text{-} 5\text{-} R) \textbf{Co-} \\ (Et_2 C_2 B_4 H_4)]^- \end{array}$	S, H, B, IR	[75]	
Linked 6,7-vertex nido, closo-[(2,3-C2B3)Co(2,3-C2B3)]2M clusters (tetradecker sandwiches)			
$\begin{array}{l} ({\rm Et_2C_2B_3H_3-4-R-5-R'}){\bf Co}({\rm C_5Me_4}){\rm -C_6H_4-} \\ ({\rm C_5Me_4}){\bf Co}[({\rm Et_2C_2B_3H_3-4-R''-5-R'''}) \ {\rm R, \ R', \ R'', \ R'''=H, \ Cl, \ Br, \ Me \ phenylene-bridged \end{array}$	S, H, B	[168]	
Other <i>nido</i> - Co C ₂ B ₃ phenylene-bridged complexes		[168]	
1,3,5-[Cp* $Co(Et_2C_2B_3H_4-5-C\equiv C)$] ₃ C ₆ H ₃ benzene-centered	S, H, B, C, IR, UV, MS	[151]	
Other <i>nido</i> - CoC_2B_3 benzene-centered complexes		[161]	
$[\textit{nido-}(Et_2C_2B_3H_4-5-Me)\textbf{Co}(\eta^5-C_5H_4)]_2$ fulvalene-bridged	S, H, B	[168]	
$\begin{array}{l} \textit{Nido, closo-}[(Et_2C_2B_3H_4\text{-}5\text{-}Me)\textbf{Co}(\eta^5\text{-}\\ C_5H_4)_2\textbf{Co}_3(Et_2C_2B_3H_2\text{-}5\text{-}Me)_2(\eta^5\text{-}C_5H_4)]_2 \\ \textit{fulvalene-bridged} \end{array}$	S, H, UV, MS(FAB)	[168]	
Other <i>nido</i> - Co C ₂ B ₃ fulvalene-bridged complexes		[168]	
6-vertex nido-1,2,3,5-CoC ₃ B ₂ clusters (diborolyl complexes)			
$Cp\textbf{Co}(Et_2H_2C_3B_2Me_2)$	S, H, B, C, MS	[40,169]	
CpCo(Et ₂ HC ₃ B ₂ Me ₂) ⁻	S, Н	[108]	
CpCo(Et ₂ MeDC ₃ B ₂ Et ₂)	S, H, B	[40]	
CpHCo($R_2R'C_3B_2R''_2$) R = Me, Et; R' = H, Me; R''=Me, Et	S, H, B, MS	[171]	
Cp Co (R ₂ R'R''C ₃ B ₂ R''' ₂) R=Me, Et; R', R''=H, Me; R'''=Me, Et	S, H, B, MS	[171]	
$(CO)_3 \textbf{Co}[cyclo-(CH_2)_6-MeC_3B_2Me_2]$	S, X, H, B, C, MS	[173]	

Compound	Information	References
$(CO)_3$ Co $(MeEt_2C_3B_2Et_2)$	S, H, B, C, MS	[174]
6-vertex nido-1,2,3,4,5-CoC ₄ B clusters		
Cp Co (H ₄ C ₄ B-Ph)- μ -SiMe ₂	S, H, B, C, IR, MS	[177]
$CpCo(H_4C_4B-R) R = Me, Ph$	S, H, B, MS	[176]
Cp Co (H ₂ D ₂ C ₄ B-Ph)	S	[176]
$(CO)_2 RCo(H_4C_4B-Ph) R = CO, PMe_3$	S	[1369]
Cp Co [H ₄ C ₄ B-N(CHMe ₂) ₂]	S, H, B	[180]
$(CO)(\mu\text{-}CO)\textbf{Co}[H_4C_4B\text{-}N(CHMe_2)_2]$	S, H, B	[180]
Nido, closo-(CO) ₃ $Mn(H_4C_4B-Me)Co(H_4C_4B-Me)$	S, He photoelectron spectra	[181]
Other <i>nido</i> -(CO) ₂ Co (3,4-R ₂ H ₂ C ₄ B-Ph) complexes		[184]
Cp Co (Ph_4C_4BR) R = Br, Ph, <i>n</i> - C_4H_9 , OH	S, H, B, IR, UV(OH), MS	[186]
$CpCo(Ph_4C_4BR) R = OMe, OSiMe_3$	S, H, MS	[186]
$(CO)_2 X Co(H_4C_4B-R) R = Me, Ph) X = Br, I$	S, H, B, IR, MS	[176]
Other <i>closo,nido</i> -L M (H ₄ C ₄ B-R) Co (H ₄ C ₄ B-R) complexes		[176]
7-vertex closo-1,2,3-CoC ₂ B ₄ clusters		
$\begin{array}{l} \textit{Nido, closo-}(Me_{2}C_{2}B_{3}H_{5})\textbf{Co}(Me_{2}C_{2}B_{4}H_{3})\text{-}\\ (\eta^{5}C_{5}H_{4})CoCp \end{array}$	Х	[166]
$Wedged\text{-}(Et_3P)_2 \textbf{CoFe}(Me_2C_2B_4H_4)_2$	S, X, H, B, P, IR	[91]
$Wedged\text{-}Cp \textbf{CoFe}[(PhCH_2)_2C_2B_4H_4]_2$	S, H, B, IR, MS	[74]
Cp_2Co^+ [Co (Et ₂ C ₂ B ₄ H ₄) ₂] ⁻	S, X, H, B, UV, MS	[75]
1,2,3-Cp Co [(Me ₃ Si) ₂ C ₂ B ₄ H ₄]	S, H, B, MS	[198]
$1,2,3\text{-}Cp\textbf{Co}[(Me_{3}Si)_{2}C_{2}B_{4}H_{3}]\text{-}\mu(5)\text{-}B_{2}H_{5}$	S, X, H, B, IR, MS	[198]
1,2,3-Cp* Co (RC ₂ B ₄ H ₅) R = Et, SiMe ₃	S, H, B, IR, MS	[126,199]
1,2,3-Cp* Co (Me ₂ C ₂ B ₄ H ₄)	S, H, B, IR, MS	[148,149]
	E	[200]
$(2,3\text{-}Et_2C_2B_4H_4)\textbf{Co}(Et_4C_4B_8H_7\text{-}OC_4H_8)$	S, X, H, B, IR, MS	[58]
$(2,3\text{-}Et_2C_2B_4H_4)\textbf{Co}(Et_4C_4B_8H_8\text{-}OC_4H_8)$	S, H, B(2d), IR, MS	[58]
1,2,3-Cp* Co (Et ₂ C ₂ B ₄ H)-4,5,6-I ₃	S, H, B, C, IR, MS	[202]
1,2,3-Cp*Co($Et_2C_2B_4$)-4,6-Me ₂ -5-R-7- O ₃ SCF ₃ R=Me, I	S, H, B, C, IR, MS	[202]
1,2,3-Cp* Co (Et ₂ C ₂ B ₄ H ₃)-7-SiMe ₃	S, H, B, UV, MS	[204]
1,2,3-Cp*Co($Et_2C_2B_4H_2$)-5-R-7-R' R=I, SiMe_3; R'=SiMe_3, H	S, H, B, C, UV(H, SiMe ₃), IR, MS	[204]
1,2,3-Cp* Co (Et ₂ C ₂ B ₄ H ₂)-5-I-7-C \equiv CR R=H, SiMe ₃	S, H, B, C, IR, MS	[202]
1,2,3-Cp* Co (Et ₂ C ₂ B ₄ H)-4,5,6-X ₃ X = Cl, I	S, H, B, C, MS	[48]
$[1,2,3-Cp*Co(C_2B_4H_5)]_2CH_2$	S, H, B, IR, MS	[126]
$1,2,3-Cp^{*}Co[(PhCH_{2})EtC_{2}B_{4}H_{4}]$	S, H, B, IR, MS	[126]

e160 APPENDIX | G Supplemental Data for Table 13-1. Selected 6- and 7-Vertex Transition Element Metallacarboranes

Compound	Information	References
1,2,3-Cp* Co [(Me ₃ Si) ₂ C ₂ B ₄ H ₄] ⁻	H (correlated), ESR	[200]
$\begin{array}{l} Cp*{\pmb{Co}}(Et_2C_2B_4H_3)\text{-}5\text{-}O(CH_2)_4\text{-}(\eta^4\text{-}C_5Me_5)\text{-}\\ {\pmb{Co}}H(Et_2C_2B_4H_3)\text{-}5\text{-}I \end{array}$	S, X, H, B, C, IR, MS	[152]
p-[1,2,3-Cp* Co (C ₂ B ₄ H ₅)CH ₂] ₂ C ₆ H ₄ phenylene-bridged	S, H, B, IR, MS	[126]
p -{1,2,3-Cp* Co [(Me ₃ Si)C ₂ B ₄ H ₄]CH ₂ } ₂ C ₆ H ₄ phenylene-bridged	H (correlated), E	[200]
$[1,2,3-(Et_2C_2B_4H_4)Co(C_5Me_4)]_2(C_6H_4)_n$ (n=1, 2) phenylene-bridged	S, H, B, IR, UV, MS	[131]
$o/m/p$ -{Cp*Co[(SiMe_3)C_2B_4H_4]CH_2}_2C_6H_4	S, H, B, IR, MS	[126]
Other $\mathbf{Co}C_2B_4$ phenylene-bridged complexes		[126]
1,3,5-[Cp* $Co(Et_2C_2B_4H_2)$ -5-X-7- C=C)] ₃ C ₆ H ₃ X = Br, I, C=CSiMe ₃ , C=CH benzene-centered	S, H, B, C, IR, UV, MS	[202]
$1,2,3\text{-}(Ph_2PCH_2)_2(Cl)\textbf{Co}(Ph_2C_2B_4H_4)$	S, H, B, C, IR, UV, MS	[206]
$(\eta^5\text{-}PhCH_2C_5Me_4)\textbf{Co}(Et_2C_2B_4H_4)$	S, H, B, IR, MS	[86]
$(\eta^5 C_5 Me_4 - C \blacksquare CSi Me_3) \textbf{Co}(Et_2 C_2 B_4 H_4)$	S, H, C, MS	[161]
1,2,3-[RC(O)(η^{5} -C ₅ H ₄)]Co(Et ₂ C ₂ B ₄ H ₄) R=Cl, OH	S, H, B,C, IR, MS	[160]
Other 1,2,3- CoC_2B_4 derivatives		[48,58,127,128,131,152,159,161,163,164]
7-vertex closo-1,7,2,3-CoC $_2B_3$ Co clusters (triple	e-decker sandwiches)	
Cp Co ($RC_2B_3H_4$) Co Cp R = Ph, SiMe ₃	S, H, B, MS	[212]
$CpCo(C_2B_3H_4-5-X)CoCp X = Br, I$	S, H, B, MS	[212]
$Cp \textbf{Co}(Me_2C_2B_3H_2\text{-}4\text{-}OEt)\textbf{Co}Cp$	S, H, B, IR, MS	[213]
$Cp \textbf{*} \textbf{Co}[(Me_3Si)_2C_2B_3H_3]\textbf{Co}Cp \textbf{*}$	S, H, B, IR, MS	[148]
$Cp*Co[Et_2C_2B_3H_2-5-C \equiv CSiMe_3]CoCp*$	S, H, B, C, IR, UV, E, MS	[151]
$(\eta^{5}-RC_{5}H_{4})\mathbf{Co}(C_{2}B_{3}H_{5})\mathbf{Co}Cp R = Me, Et,$ SiMe ₃	S, H, B, MS	[212]
$(\eta^{5}-NC_{4}Me_{4})Co(Et_{2}C_{2}B_{3}H_{2}X)CoCp^{*}X = H, Br, Cl$	S, H, B, IR, UV, MS	[129]
$(\eta^{5}\text{-}PC_{4}Me_{4})_{2}\textbf{Co}_{2}(Et_{2}C_{2}B_{3}H_{3}) \text{ phospholyl}$	S, H, B, P, IR, UV, E, MS	[129]
Other (phospholyl) $Co(C_2B_3)M$ triple-decker complexes		[129]
Other $Co(2,3-C_2B_3)M$ triple-decker complexes		[88,148]
7-vertex closo-1,7,2,3-CoC ₂ B_3M clusters (triple	-decker sandwiches)	
$Cp*{\textbf{Co}}(Et_2C_2B_3Br_3){\textbf{Ta}}Cl_2Cp$	S, X, H, B, C, MS	[25]
$Cp*{\textbf{Co}}(Et_2C_2B_3HI_2){\textbf{Ta}}CI_2Cp$	S, H, B, MS	[20,25]
$Cp*Co(Et_2C_2B_3H_3)TaCpLL' L = Me, CH_2Ph; L' = CI, Me, CH_2Ph, CH_2CMe_3$	S, X(Me $_2$, CH $_2$ Ph; Cl), H, B, C, IR, UV, MS	[20]
$CpCl_2 \textbf{Ta}(Et_2C_2B_3Br_3) \textbf{Co}Cp^{\textbf{*}}$	S, X, H, B, C, MS	[25]
$CpCl_2 \textbf{Ta}(Et_2C_2B_3HI_2) \textbf{Co}Cp^*$	S, H, B, MS	[20,25]
CpLL' Ta (Et ₂ C ₂ B ₃ H ₃) Co Cp* L=Me, CH ₂ Ph; L'=Cl, Me, CH ₂ Ph, CH ₂ CMe ₃	S, X(Me_2, CH_2Ph; Cl), H, B, C, IR, UV, MS	[20]
$CpCl_2 \textbf{Ta}(Et_2C_2B_3Br_3) \textbf{Co}Cp^*$	S, X, H, B, C, MS	[25]

Compound	Information	References
$CpCl_2 Ta(Et_2C_2B_3Hl_2)CoCp^*$	S, H, B, MS	[20,25]
CpLL' Ta (Et ₂ C ₂ B ₃ H ₃) Co Cp* L=Me, CH ₂ Ph; L'=Cl, Me, CH ₂ Ph, CH ₂ CMe ₃	S, X(Me ₂ , CH ₂ Ph; Cl), H, B, C, IR, UV, MS	[20]
$Cp^{*}\textbf{Co}(Et_{2}C_{2}B_{3}H_{2}\text{-}5\text{-}CH_{2}Ph)\textbf{Mo}(CO)_{4}$	S, X, H, IR, UV, E, MS	[31]
$\label{eq:constraint} \begin{split} &[(\eta^{5}\text{-}NC_{4}Me_{2}R_{2})\textbf{Co}(Et_{2}C_{2}B_{3}H_{3})\textbf{Ru}(p\text{-}CHMe_{2}C_{6}H_{4}Me) \ R = Me, \ H \end{split}$	S, H, B, IR, UV, E, MS	[129]
$Cp*\mathbf{Rh}(Et_2C_2B_3H_2-4-R)\mathbf{Co}Cp*R=H, CI$	S, H, B, IR, E(H), MS	[133]
7-vertex closo-1,7,2,4-CoC ₂ B ₃ Co clusters (triple	e-decker sandwiches)	
Cp Co $(2,4-RC_2B_3H_4)$ Co Cp R=Ph, SiMe ₃	S, H, B, MS	[212]
$(\eta^{5}-RC_{5}H_{4})Co(2,4-C_{2}B_{3}H_{5})CoCp R = Me, Et, SiMe_{3}$	S, H, B, MS	[212]
7-vertex closo-1,7,2,3,5-CoC ₃ B ₂ M clusters (dib	orolyl triple-decker sandwiches)	
$Cp\textbf{Co}(Et_2MeC_3B_2Et_2)\textbf{Co}Cp^+$	S, H, B, MS	[100]
$Cp \textbf{Co}(Me_{3}C_{3}B_{2}Me_{2})\textbf{M}(C_{8}H_{12}) \ \textbf{M} \!=\! R\textbf{h}, \ \textbf{Ir}$	S, H, B	[220]
Cp Co (Me ₃ C ₃ B ₂ Me ₂) M Br ₂ M =Rh, Ir	S, H, B	[220]
$Cp\textbf{Co}(Me_3C_3B_2Me_2)\textbf{M}Cp \textbf{ M} = Rh, Ir$	S, H, B	[220]
$\begin{array}{l} 1,\!7,\!2,\!3,\!5\text{-}Cp\textbf{Co}(Me_3C_3B_2Me_2)\textbf{RuL}^{+} L\!=\!C_6H_6,\\ C_6Me_6,\ MeC_6H_4CHMe_2,\ \eta_6\text{-}C_7H_8 \end{array}$	S, X(C ₆ H ₆ , C ₆ Me ₆), H, B, U(CoCp), E	
$CpCo[(CH_2=CMe)(CHMe_2)RC_3B_2Me_2]CoCp$ R=Me, MeC=CH ₂ , CHMe ₂	S, H, E, MS	[172]
$CpCo[(H_4C_4)RC_3B_2Me_2]CoCp R = Me, \\ MeC = CH_2, CHMe_2, CMe_2C_5H_5CoCp$	S, X(CHMe ₂ , CMe ₂ C ₅ H ₅ CoCp), H, E, MS	[172]
$\{Cp\textbf{Co}[(H_4C_4)(CHMe_2)C_3B_2Me_2]\textbf{Co}Cp\}^+$	S, H, B, C, MS	[172]
$CpCo[(H_4C_4)RC_3B_2Me_2]CoCp R = cyclo-C_5H_7$, cyclo-C_5H9	S, X, H, MS	[172]
$Cp \textbf{Co}(Me_2HC_3B_2Me_2)\textbf{Fe}Cp$	E	[102]
$[Cp \textbf{Co}(Et_2HC_3B_2Me_2)\textbf{Fe}Cp]^+$	S, H, MAG, Mössbauer	[100]
$[CpCo(Et_2MeC_3B_2Et_2)FeCp]^{n+} n=+1, -1$	ESR	[100]
$Cp \textbf{Co}(Me_3C_3B_2Me_2)\textbf{Ru}(C_5R_5)$	S, X(H, Me), B, E, UV	[222]
$[Cp\textbf{Co}(Et_2MeC_3B_2Et_2)\textbf{Ni}Cp]^-$	S, ESR	[100]
$Cp \textbf{Co}(Et_2HC_3B_2Me_2)\textbf{Ni}(C_3H_5)$	S, H, B, MS	[223]
CpCo(Et ₂ HC ₃ B ₂ Me ₂)NiCp	S, X, H, MS	[100]
$[Cp\textbf{Co}(Et_2MeC_3B_2Et_2)\textbf{Ni}(CO)]_2$	S, IR, MS	[100]
	S, H, B, MS	[103]
$Cp \textbf{Co}(Et_2 MeC_3 B_2 Et_2) \textbf{Ni}(CO)(\mu\text{-}CO)_2 FeCp$	S, IR, MS	[100]
7-vertex closo,nido-CpCo $(2,3,5-C_3B_2)$ CoL L = b	orane or thiaborane (diborolyl-borane tri	ple-decker sandwiches)
$Cp \textbf{Co}(MeEt_2C_3B_2Et_2)\textbf{Co}(S_2B_9H_9)$	S, H, B, MS	[225]
$Cp \textbf{Co}(\text{MeEt}_2C_3B_2\text{Et}_2)\textbf{Co}(S_2B_6\text{H}_8)$	S, X, H, B, C, MS	[225]
7-vertex closo,nido-CpCo(2,3,5-C ₃ B ₂)Co(2,3-C ₃	(B_y) (diborolyl-nido-carborane triple-deck	er sandwiches)
$Cp \textbf{Co}(MeEt_2C_3B_2Et_2)\textbf{Co}(C_2B_5H_7)$	S, H, B, MS	[226]
$Cp \textbf{Co}(MeEt_2C_3B_2Et_2)\textbf{Co}(C_2B_9H_{11})$	S, X, H, B, E, MS	[227]

e162 APPENDIX | G Supplemental Data for Table 13-1. Selected 6- and 7-Vertex Transition Element Metallacarboranes

Compound	Information	References
$Cp \textbf{Co}(MeEt_2C_3B_2Et_2)\textbf{Rh}(C_2B_7H_9)$	S, H, B, MS	[226]
$Cp\textbf{Co}(\text{Et}_2MeC_3B_2\text{Et}_2)\textbf{Fe}(\text{Et}_2C_2B_3H_5)$	S, MS	[98]
$Cp\textbf{Co}(\text{Et}_2\text{MeC}_3\text{B}_2\text{Et}_2)\textbf{Fe}[(\text{PhCH}_2)_2\text{C}_2\text{B}_3\text{H}_5]$	S, MS	[98]
$Cp \textbf{Co}(MeEt_2C_3B_2Et_2) \textbf{Ni}(8\text{-}Me\text{-}2,3,5\text{-}C_3B_7H_9)$	S, X, H, B, MS	[99]
7-vertex closo, closo-Co(2,3-C ₂ B ₃)M(2,3-C ₂ B ₃)M	clusters (tetradecker sandwiches)	
$Cp*\textbf{Co}(Et_2C_2B_3H_4\text{-}5\text{-}Cl)\textbf{Co}(Et_2C_2B_3H_4\text{-}5\text{-}Cl)\textbf{-}\\\textbf{Co}Cp*$	s, h, uv, ms	[218]
$\label{eq:constraint} \begin{split} &[(\eta^6\text{-}\text{MeC}_6\text{H}_4\text{CHMe}_2)\text{Ru}(\text{Et}_2\text{C}_2\text{B}_3\text{H}_2\text{-}\text{5-X})]_2\text{Co}\\ &X=\text{Me},\ \text{Cl} \end{split}$	S, X(Me), H, IR, UV, MS	[114]
$[(\eta^6\text{-}\text{MeC}_6\text{H}_4\text{CHMe}_2)\textbf{Ru}(\text{Et}_2\text{C}_2\text{B}_3\text{Me}_3)]_2\textbf{Co}$	s, ir, uv, ms	[114]
Other Co-Ru tetradecker sandwiches		[114]
$\label{eq:constraint} \begin{split} &[(\eta^6\text{-}MeC_6H_4CHMe_2)\mathbf{Ru}(Et_2C_2B_3H_3)\mathbf{Co}\text{-}\\ &(Et_2C_2B_3H_3)\mathbf{Co}Cp \end{split}$	S, H, B, IR, MS, E	[135]
$Cp^{*}Co(Et_{2}C_{2}B_{3}H_{4}\text{-}5\text{-}Cl)\mathbf{Rh}H(Et_{2}C_{2}B_{3}H_{4}\text{-}5\text{-}Cl)\text{-}MCp^{*}M = Ir, Co$	s, h, uv, ms	[218]
$Cp*\textbf{Co}(Et_2C_2B_3H_4\text{-}5\text{-}Cl)\textbf{Ir}(Et_2C_2B_3H_4\text{-}5\text{-}Cl)\textbf{-}\\\textbf{Co}Cp*$	s, h, uv, ms	[218]
$\label{eq:constraint} \begin{split} & [Cp^* \textbf{Co}(Et_2C_2B_3H_2\text{-}5\text{-}X]_2\textbf{Ni} \ X \!=\! CI, \ Br, \\ & CH_2C \!\equiv\! CMe \end{split}$	S, Н	[229]
$[Cp*\textbf{Co}(Et_2C_2B_3H-4,5-Cl_2]_2\textbf{Ni}$	S, H, B, C, E, Ms	[138]
$[Cp^*\textbf{Co}(Me_2C_2B_3H_2\text{-}5\text{-}Me]_2\textbf{Ni}$	S, H, B, IR, MS	[148]
$[Cp^{*}\textbf{Co}(Et_{2}C_{2}B_{3}FCl_{2}]_{2}\textbf{Ni}$	S(electrochem), H, F, E, MS	[138]
$[Co(2,3,5-C_3B_2)]_2M$ and $[M(2,3,5-C_3B_2)]_2Co$ (dib	orolyl tetradecker sandwiches)	
$[Cp\textbf{Co}(MeEt_2C_3B_2Et_2)]_2\textbf{Ni}$	S, H, E, MS	[227]
$[Cp\textbf{Co}(Et_2HC_3B_2Me_2)]_2\textbf{Ni}^{2-}$	Н	[108]
Rhodium		
6-vertex nido-1,2,3,5-RhC ₃ B ₂ clusters (diboroly	l complexes)	
$[\textit{nido-}\mu\text{-}Cl\text{-}\textbf{Rh}(HMeEt_2C_3B_2Et_2)]_2$	S, H, B, MS	[235]
Nido-Cp Rh (HMeEt ₂ C ₃ B ₂ Et ₂)	S, H, B, MS	[235]
Nido-Cp Rh (Ph ₃ P-Au-MeEt ₂ C ₃ B ₂ Et ₂)	S, H, B, P, MS	[170,235]
7-vertex closo-1,2,3,5-RhC ₃ B ₃ clusters		
1,2,3,5-(OC) ₂ Rh (Et ₃ C ₃ B ₃ Et ₃)	S, X, H, B, C, P, MS	[1383]
7-vertex closo-1,7,2,3,5-CoC ₃ B ₂ Rh clusters (dib	orolyl triple-decker sandwiches)	
$Cp \textbf{Co}(Me_3C_3B_2Me_2)\textbf{Rh}(C_8H_{12})$	S, H, B	[220]
$Cp \textbf{Co}(Me_3C_3B_2Me_2)\textbf{Rh}Br_2$	S, H, B	[220]
7-vertex closo, closo- $M(C_3B_2)Rh(C_xB_y)M'$ and R_1	$h(C_2B_3)M(C_3B_2)M'$ tetradecker sandwiches	s
$Cp*\text{Ir}(\text{Et}_2\text{C}_2\text{B}_3\text{H}_4\text{-}5\text{-}\text{Cl})\text{Rh}\text{H}(\text{Et}_2\text{C}_2\text{B}_3\text{H}_4\text{-}5\text{-}\text{Cl})\text{-}\text{Ir}\text{Cp}*$	S, H, UV, MS	[218]
$Cp*lr(Et_2C_2B_3H_4-5-Cl)RhH(Et_2C_2B_3H_4-5-Cl)-CoCp*$	S, H, UV, MS	[218]
$Cp^{*}\textbf{Co}(Et_{2}C_{2}B_{3}H_{4}\text{-}5\text{-}Cl)\textbf{Rh}H(Et_{2}C_{2}B_{3}H_{4}\text{-}5\text{-}Cl)\text{-}\textbf{Co}Cp^{*}$	S, H, UV, MS	[218]

Compound	Information	References	
Nickel			
6-vertex nido-1,2,3,5-NiC ₃ B ₂ clusters (diborolyl complexes)			
Cp Ni [cyclo-(CH ₂) ₆ MeHC ₃ B ₂ Me ₂]	S, X, H, B, C, MS	[173]	
$(C_8H_{12})Ni[Et_2(Me_2CH)C_3B_2Me_2]$	S, H, B, C, MS	[238]	
$CpNi(Et_2MeC_3B_2Et_2)$	S, H, B	[239]	
	Х	[240]	
$(Et_3HC_3B_2Et_2)_2$ Ni	S, X, B, C	[1384]	
7-vertex closo-1,2,4-NiC ₂ B ₄ clusters			
$(Ph_2PCH_2)_2 Ni(C_2B_4H_6)$	S, H, B, IR, MS	[142]	
	S, H, B, IR	[1364]	
$(TMEDA)\mathbf{Ni}[(Me_3Si)_2C_2B_4H_4]$	S, IR, ESR	[90]	
7-vertex closo-1,2,3,5-NiC ₃ B ₃ clusters			
$(C_3H_5)\textbf{Ni}[Et_2(CHMe_2)C_3B_3EtR_2] R=Me, Et$	S, H, B, C(Et), MS	[210]	
$CpNi(\mu\text{-}CO)_2 \textbf{Ni}[(CHMe_2)_2 MeC_3 B_3 Et_3]$	S, H, B, C, IR, MS	[210]	
7-vertex closo-1,7,2,3,5-NiC ₃ B ₂ M clusters (dibe	orolyl triple-decker sandwiches)		
$(C_3H_5)_2\textbf{Ni}(Me_2RC_3B_2Me_2)\textbf{Ni}(C_3H_5)$	S, H, B, C, MS	[245]	
$CpNi(Et_2HC_3B_2Me_2)NiCp$	S, X, MS	[100]	
	H(correlated), E	[242]	
$[Cp\mathbf{Ni}(Et_2HC_3B_2Me_2)\mathbf{Ni}Cp]^-$	S, H	[100]	
$(C_3H_5)\textbf{Ni}(Me_2HC_3B_2Me_2)\textbf{Ni}(C_3H_5)_2$	S, H, B, MS	[248]	
$\begin{array}{l}(Et_2HC_3B_3Me_3)\mathbf{Ni}(Et_2HC_3B_2Me_2)\mathbf{Ni}\\(Et_2HC_3B_3Me_3)\end{array}$	S, H, ESR, E	[242]	
$\begin{array}{l}(Me_2HC_3B_3Me_3)\mathbf{Ni}(Me_2HC_3B_2Me_2)\mathbf{Ni}\\(Me_2HC_3B_3Me_3)\end{array}$	s, h, b, ms	[241]	
$Cp \textbf{Co}(Et_2 MeC_3 B_2 Et_2) \textbf{Ni}(CO)(\mu\text{-}CO)_2 FeCp$	S, IR, MS	[100,103]	
	Н	[103]	
$(CO)_3 \textbf{Fe}(Et_2 MeC_3 B_2 Me_2) \textbf{Ni}(CO)(\mu\text{-}CO)_2 FeCp$	S, H, B, IR, MS	[103]	
$(CO)_3 \textbf{Fe}(Et_2HC_3B_2Me_2)\textbf{Ni}Cp$	S, H, B, IR, MS	[103]	
$(CO)_3 \textbf{Fe}(Et_2 MeC_3 B_2 Me_2) \textbf{Ni}Cp$	S, H, IR, MS	[103]	
$[Cp\textbf{Co}(Et_2MeC_3B_2Et_2)\textbf{Ni}(CO)]_2$	S, IR, MS	[100]	
	S, H, B, MS	[103]	
$[Cp\mathbf{Ni}(Et_2MeC_3B_2Et_2)\mathbf{Co}Cp]^-$	S, ESR	[100]	
$Cp \textbf{Co}(Et_2 MeC_3 B_2 Et_2) \textbf{Ni}(CO)(\mu\text{-}CO)_2 \textbf{Fe}Cp$	S, IR, MS	[100]	
7-vertex closo-Ni(2,3,5-C ₃ B ₂) $M(C_xB_y)$ (diborolyl-carborane triple-decker sandwiches)			
$Cp \textbf{Co}(Et_2 MeC_3 B_2 Et_2) \textbf{Ni}(Et_2 C_2 B_4 H_4) \textbf{Fe}(\eta^5 - C_9 H_7)$	S, H, B, IR, MS, E	[54]	
$Cp \textbf{Co}(Et_2HC_3B_2Me_2) \textbf{Ni}(Et_2C_2B_4H_4) \textbf{Fe}Cp^*$	S, H, B, IR, MS	[54]	
7-vertex closo, closo- $M(C_2B_3)Ni(C_2B_3)M'$ and $Ni(C_2B_3)M(C_2B_3)M'$ tetradecker sandwiches			
$[(Me_2HC_3B_3Me_3)\mathbf{Ni}(Me_2HC_3B_2Me_2)]_2\mathbf{Ni}$	S, H, MS	[241]	
$[(\eta^6\text{-}\text{MeC}_6\text{H}_4\text{CHMe}_2)\textbf{Ru}(\text{Et}_2\text{C}_2\text{B}_3\text{Me}_3)]_2\textbf{Ni}$	S, IR, UV, MS	[114]	

e164 APPENDIX | G Supplemental Data for Table 13-1. Selected 6- and 7-Vertex Transition Element Metallacarboranes

Compound	Information	References
$[Cp*Co(Et_2C_2B_3H_2-5-X]_2Ni X = CI, Br, CH_2C \equiv CMe$	S, H	[229]
$[(E t_2 C_2 B_3 H_2 M e) \textbf{CoH} (E t_2 C_2 B_4 H_4)]_2 \textbf{Ni}$	S, UV, MS	[128]
7-vertex [closo-M(2,3,5-C ₃ B ₂)] ₂ Ni diborolyl tetr	adecker sandwiches	
$[Cp\textbf{Co}(Et_2HC_3B_2Me_2)]_2\textbf{Ni}^{2-}$	Н	[108]
$[Cp\textbf{Co}(MeEt_2C_3B_2Et_2)]_2\textbf{Ni}$	S, H, E, MS	[227]
$[Cp\textbf{Co}(MeEt_2C_3B_2Et_2)]_2\textbf{Ni}$	S, H, E, MS	[227]
$\{CpNi[(H_4C_4)MeC_3B_2Me_2]\}_2Ni$	S, X, H	[249]
$[(C_3H_5)\mathbf{Ni}(MeEt_2C_3B_2Et_2)]_2\mathbf{Ni}$	S	[250]
Platinum		
6-vertex nido-1,2,3,5-PtC ₃ B ₂ clusters (diboroly)	complexes)	
$(E t_2 M e C_3 B_2 E t_2)_2 \mathbf{P} \mathbf{t}$	S, H, B, C, IR, MS	[253]
$[(E t_2 Me C_3 B_2 E t_2)_2 \mathbf{P} t]^{2-}$	S, H, B, C	[253]
$(C_8H_{13})\textbf{Pt}(Et_2MeC_3B_2Et_2)$	S, X, H, B, C, MS	[255]
$(Et_2MeHC_3B_2Me_2)_2$ Pt	S, X, H(variable T), B, C	[1384]
7-vertex commo-[(2,3,5-C ₃ B ₂)M] ₂ Pt clusters (di	borolyl tetradecker sandwiches)	
(C_8H_{13}) Pt $(Et_2MeC_3B_2Et_2)$ Pt (C_8H_{12})	S, H, B, MS	[255]
(C_8H_{13}) Pt $(Me_2HC_3B_2Me_2)$ Pt (C_8H_{12})	S, X, H, B, C, MS	[255]
Lanthanide Metals		
7-vertex LnC_2B_4 clusters		
$\begin{array}{l} \mu, closo-[\textbf{Gd}(SiMe_3)_2C_2B_4H_4]_3[\mu_2\text{-Li}-\\ (SiMe_3)_2C_2B_4H_4]_3[\mu_3\text{-OMe})[\mu_2\text{-Li}-\\ (OC_4H_8)]_3(\mu_3\text{-O}) \end{array}$	S, X, IR	[259]
$\{Cl_2 \text{\bf Er}[2,3\text{-}(SiMe_3)_2 C_2 B_4 H_4]_2 Li_2 (TMEDA)_2\}^-$	S, X, IR, MAG	[260]
$ \{ [2,3-(SiMe_3)_2C_2B_4H_4] \textbf{Er} [2,4-(SiMe_3)_2C_2B_4H_4] \}^{2-} $	S, X, IR, MAG	[260]
$\label{eq:constraint} \begin{split} &[(SiMe_3)_2C_2B_4H_4]_2\text{Ln}Cl_2(\mu\text{-H})_3\text{Li}(\text{TMEDA})\\ &(\mu\text{-H})_2(\text{TMEDA})\ \text{Ln}=\text{Sm},\ \text{Gd},\ \text{Tb},\ \text{Dy},\ \text{Ho} \end{split}$	S, X, H(Sm), B(Sm), C(Sm), Li(Sm), IR, MAG(Sm, Gd, Dy, Ho)	[262]
$\begin{array}{l} (TMEDA)Li(\mu\text{-}Cl)_2 Ho[2,4-\\ (SiMe_3)_2 C_2 B_4 H_4]_2 (\mu\text{-}H)_4 HoCl_2 (TMEDA)_2 \end{array}$	S, X	[263]
$\{[(SiMe_{3})_{2}C_{2}B_{4}H_{4}]_{2}\textbf{Ho}Cl_{2}\cdot Li_{2}(TMEDA)_{2}\}^{-}$	Х	[264]
$\begin{array}{l} ({\sf Me}_3{\sf COH})_2({\sf Me}_3{\sf CO}){\pmb Sm}[({\sf SiMe}_3)_2{\sf C}_2{\sf B}_4{\sf H}_4]\mbox{-}\mu\mbox{-}\\ (4,5)\mbox{-}{\sf Li}({\sf OC}_4{\sf H}_8){\sf Cl} \end{array}$	S, X, H, B, C, IR	[265]
$\label{eq:Li} \begin{array}{l} \text{Li}(\text{TMEDA})_2^{+}\{[(\text{SiMe}_3)_2\text{C}_2\text{B}_4\text{H}_4]_2\text{-}\\ \textbf{Ce}\text{Cl}_2\text{\cdot}\text{Li}_2(\text{TMEDA})_2\}^{-} \end{array}$	S, X, IR,MAG	[266]
$\label{eq:states} \begin{array}{l} \textit{Nido-2,4-(SiMe_3)_2C_2B_4H_4-}\mu(5,6)\text{-}H_2\text{-}Ln-\\ [(SiMe_3)_2C_2B_4H_4]_2 \ Ln=Er, \ Dy \end{array}$	X, IR	[267]
$\{[2,4\text{-}(SiMe_3)_2C_2B_4H_4]_2\textbf{Lu}\}^- Na(OC_4H_8)_2^{+}$	S, X, H, C, IR, MAG	[268]
	S, X, I	[270]
Na ⁺ ₃ [(2,4-(SiMe ₃) ₂ C ₂ B ₄ H ₄] ₂ Ln[μ -5,6- <i>nido</i> -2,4-(SiMe ₃) ₂ C ₂ B ₄ H ₄] ³⁻ Ln = Dy, Er	S, X, IR	[271]
$O\{(OC_4H_8) \textbf{Ho}[2,4\text{-}(SiMe_3)_2C_2B_4H_4]\}_4Cl_2$	S, X, IR, MAG	[272]

Compound	Information	References	
$\{1,2,3-(THF)_m BrLn[(Me_3Si)_2C_2B_4H_4]\}_2$ ·THF Ln=Ce, Pr; $m=1, 2$	S, IR	[10]	
$\{1,2,3-(THF)Br \textbf{La}[(Me_{3}Si)_{2}C_{2}B_{4}H_{4}]\}_{2}$	S, X, H, B, C, IR	[10]	
$\{1,2,3\text{-}(THF)_2Cl\textbf{Lu}[(Me_3Si)_2C_2B_4H_4]\}_2\text{-}THF$	S, X, H, B, C, IR	[10]	
$ \{ [(Me_3Si)MeC_2B_4H_4] - 1, 2, 3 - (\mu-H)Ln[(Me_3Si) - RC_2B_4H_4] \}_2 \cdot (THF)_n Ln = Nd, Ho, Er, Gd; R = Me, SiMe_3 $	S, X(Nd), IR	[10]	
1,2,3-CpLn[(Me ₃ Si) ₂ C ₂ B ₄ H ₄]·(THF) _n Ln = Tb, Dy, Er; $n=2$, 3	S, IR	[10]	
$(\eta^8\text{-}C_8H_8)\textbf{Gd}[(\text{Me}_3\text{Si})_2\text{C}_2B_4H_4](\mu\text{-}H)\text{-}\text{THF}$	S, X, IR	[10]	
$[Me_2N(CH_2)_2NMe_2]Cl\boldsymbol{D}\boldsymbol{y}[(Me_3Si)_2C_2B_4H_4]$	S, X	[276]	
Theoretical Studies			
Molecular and electronic structure calculations			
$1,2,3$ - Cr $(C_2B_4H_6)^{2-}$	MNDO	[30]	
$1,2,4-(PH_3)_2$ Pt(C ₂ B ₄ H ₆)	Extended Hückel, slip-distortion	[277]	
Nido, closo-(CO) ₃ Mn (H ₄ C ₄ B-Me) Co (H ₄ C ₄ B-Me)	INDO <i>, ab initio</i> (He photoelectron spectra)	[181]	
$[CpCo(2,3,5-C_3B_2R_5)]_2MM = Cr, Mn, Fe, Co, Ni, Cu, Zn diborolyl tetradecker sandwiches$	Extended Hückel	[278]	
<i>Nido</i> - M [Cp Co (2,3,5-C ₃ B ₂ H ₅)] ₂ M = Cr , Mn , Fe , Co , Ni , Cu , Zn diborolyl double-decker sandwiches	Extended Hückel	[278]	
$1,2,4-H_n$ Fe (Et ₂ C ₂ B ₄ Et ₄) _{n-2}	DFT: geometry, NMR	[95]	
Nido-1,2,3,5-Cp Fe (C ₃ B ₂ H ₅) diborolyl complex	Extended Hückel	[62]	
<i>Nido</i> -1,2,4,5-Cp* ₂ $\mathbf{Ru}_2(Me_2C_2B_2H_5)(\mu$ -BH ₂)	DFT: electronic and molecular structures; ionization potentials; reactions with alkyne analogues	[1381]	
Nido-Cp* ₂ Ru ₂ (Me ₂ C ₂ B ₂ H ₆) (alternative structure)	DFT: electronic and molecular structures; ionization potentials; reactions with alkyne analogues	[1381]	
1,2,4,5-Cp* ₂ Ru ₂ (Me ₂ C ₂ B ₃ H ₃)	DFT: electronic and molecular structures; ionization potentials; reactions with alkyne analogues	[1381]	
1,7,2,3,5-Cp* ₂ Ru ₂ [Me ₃ C ₃ B ₂ R(=CH ₂)] R=Me, Cl	DFT: $B = CH_2$ bending	[1372]	
$(CO)_{12}HRu_4(PhCBH)-\mu-CHPh$	Fenske-Hall	[112]	
$HCp \mathbf{W}(CO)_{11} \mathbf{Ru}_3(PhCBH)\text{-}\mu\text{-}CHPh$	Fenske-Hall	[112]	
1,7,2,3,5-Cp Co (Me ₃ C ₃ B ₂ Me ₂)MCp' ⁺ Cp'=Cp, Cp* $M=Co$, Rh, Ir	DFT: geometry, electrochemistry	[1379]	
$\begin{array}{l} 1,\!7,\!2,\!3,\!5\text{-}Cp \textbf{Co}(Me_3C_3B_2Me_2)\textbf{RuL}^{+} L\!=\!C_6H_6,\\ C_6Me_6,\ MeC_6H_4CHMe_2,\ \eta_6\text{-}C_7H_8 \end{array}$	DFT: geometry, electrochemistry	[1379]	
$\begin{array}{l} (\eta^6\text{-}C_6H_6) \textbf{Fe}(\text{Et}_2C_2B_4H_3)\text{-}5\text{-}(C_6H_5)\textbf{Fe}\text{-}\\ (\text{Et}_2C_2B_4H_4) \end{array}$	DFT, PM3	[78]	
$[(\eta^6\text{-}C_6H_6)\textbf{Fe}(\text{Et}_2C_2B_4H_3)\text{-}5]_2$	DFT, PM3	[78]	

e166 APPENDIX | G Supplemental Data for Table 13-1. Selected 6- and 7-Vertex Transition Element Metallacarboranes

Compound	Information	References
$\begin{array}{l} (\eta^6 \hbox{-} C_6 H_6) \mbox{Fe}(Et_2 C_2 B_4 H_3) \hbox{-} 5 \hbox{-} (C_6 H_5) \mbox{Fe} \hbox{-} \\ (Et_2 C_2 B_4 H_3) \hbox{-} 5' \hbox{-} (C_6 H_5) \mbox{Fe}(Et_2 C_2 B_4 H_4) \end{array}$	DFT, PM3	[78]
1,7,2,3-Cp ₂ Co ₂ (C ₂ B ₃ H ₅)	Extended Hückel	[88,284]
$Cp\mathbf{Co}(H_4C_4B-R) R = H$, Me	INDO, <i>ab initio</i> (He photoelectron spectra)	[285]
1,2,7-Cp Co (C ₂ B ₄ H ₅)-7-(CH=CH-C ₆ H ₄ NO ₂)	Second-order NLO properties, MOs	[286]
$1,2,3-[(O_2N-C_6H_4-CH=CH)C_5H_4]$ Co - $(C_2B_4H_6)$	Second-order NLO properties, MOs	[286]
$1,2,7-[(O_2N-C_6H_4-CH=CH)C_5H_4]$ Co - $(C_2B_4H_6)$	Second-order NLO properties, MOs	[286]
$Cp \textbf{Co}(Et_2HC_3B_2Me_2)\textbf{Co}Cp$	INDO	[100]
nido, closo- $M_2(H_4C_4B-Me)_3 M = Co, Rh$	INDO, <i>ab initio</i> (He photoelectron spectra)	[285]
$Cp \textbf{Ni}(H_3C_3B_2H_2) \textbf{Ni}Cp \ diborolyl \ triple-decker sandwich$	Fenske-Hall	[249]
$CpM(C_3B_2R_5)CoCp^{n+}M = Fe, Ni; n=0,1$ diborolyl triple-decker sandwich	Extended Hückel	[284]
$CpNi(C_3B_2R_5)NiCp^{n+} n=1, 0, -1$	Extended Hückel	[284]
Cp Ni ($Et_2RC_3B_2Et_2$) Co Cp	INDO	[100]
$[Cp\textbf{Ni}(H_3C_3B_2H_2)]_2\textbf{Ni}$ diborolyl tetradecker sandwich	Fenske-Hall	[249]
$(E t_3H C_3B_2E t_2)_2\mathbf{N} \mathbf{i}$	DFT: molecular structure	[1384]
$(Et_2MeHC_3B_2Me_2)_2$ Pt	DFT: molecular structure	[1384]

^a Metals incorporated into the cluster framework are shown in **boldface**. ^bS, synthesis; X, X-ray diffraction; H, ¹H NMR; B, ¹¹B NMR; C, ¹³C NMR; F, ¹⁹F NMR; P, ³¹P NMR; Li, ⁷Li NMR; Pt, ¹⁹⁵Pt 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.