

## Appendix A

# Supplemental Data for Table 7-1. *nido*-CB<sub>10</sub>H<sub>13</sub><sup>-</sup>, *nido*-CB<sub>10</sub>H<sub>12</sub><sup>2-</sup>, and *nido*-CB<sub>10</sub>H<sub>11</sub><sup>3-</sup> Derivatives

Compound	Information <sup>a</sup>	References
<b>Synthesis and Characterization</b>		
<i>No substituents on boron</i>		
7-(Me <sub>3</sub> CNH)CB <sub>10</sub> H <sub>12</sub> <sup>-</sup>	S, X, H, B	[290]
7-PhCB <sub>10</sub> H <sub>12</sub> <sup>-</sup>	S, H, B, C	[17]
7-[( <i>cyclo</i> -C <sub>6</sub> H <sub>11</sub> )H <sub>2</sub> N]CB <sub>10</sub> H <sub>12</sub>	S, H, B, C	[2]
7-( <i>cyclo</i> -C <sub>6</sub> H <sub>11</sub> )Me <sub>2</sub> N-CB <sub>10</sub> H <sub>12</sub>	S, X, H, B, C	[2]
7-(Me <sub>3-n</sub> H <sub>n</sub> N)CB <sub>10</sub> H <sub>12</sub>	S, H, B, IR	[14]
7-(Et <sub>3-n</sub> H <sub>n</sub> N)CB <sub>10</sub> H <sub>12</sub>	S, H, B, IR	[14]
7-(H <sub>2</sub> PrN)CB <sub>10</sub> H <sub>12</sub>	S	[8]
<i>D or C-containing substituents on boron</i>		
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>6</sub> D <sub>5</sub> -9-Cl	S, H, B (2d), MS, IR	[22]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>6</sub> D <sub>4</sub> -6,9-Cl <sub>2</sub>	S, H, B (2d), MS, IR	[22]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>6</sub> D <sub>4</sub> -6,9-Cl <sub>2</sub>	S, H, B (2d), MS, IR	[22]
7-(MeD <sub>2</sub> N)CB <sub>10</sub> H <sub>12-n</sub> D <sub>n</sub> , (EtD <sub>2</sub> N)CB <sub>10</sub> H <sub>12-n</sub> D <sub>n</sub>	S, MS	[10]
7-(H <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> -8-CH <sub>2</sub> Ph	S, H, B	[13]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> -8-CH <sub>2</sub> Ph	S, H, B(2d), MS	[13]
7-MeCB <sub>10</sub> H <sub>11</sub> -(μ-9,10)-MeCH <sup>-</sup>	S, X	[35]
7-PhCB <sub>10</sub> H <sub>11</sub> -(μ-9,10)-PhCH <sup>-</sup>	S, X	[38]
[—(CH <sub>2</sub> ) <sub>n</sub> -NH(CB <sub>10</sub> H <sub>12</sub> )—] <sub>n</sub> polymers	S, H, B, C, IR (diffuse reflectance)	[43]
<i>N- or P-containing substituents on boron</i>		
7-[ <i>bicyclo</i> -7,8,10-(CH <sub>2</sub> ) <sub>3</sub> CHB=NEt <sub>2</sub> ]CB <sub>10</sub> H <sub>9</sub> <sup>-</sup>	S, X, H, B, C, IR	[576]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>10</sub> -μ-PMe	S, H, B, IR	[41]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>10</sub> -μ-PEt	S, H, B, IR	[41]
7-CB <sub>10</sub> H <sub>12</sub> -8-[(Ph <sub>2</sub> P-η <sup>5</sup> -C <sub>5</sub> H <sub>4</sub> )Fe(η <sup>5</sup> -C <sub>5</sub> H <sub>4</sub> PPh <sub>2</sub> )]	S, H, B, C, P, MS, IR	[31]

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Compound	Information	References
<b>O- or S-containing substituents on boron</b>		
7-CB <sub>10</sub> H <sub>11</sub> -9-Me-10-OH <sup>-</sup>	S, B(2d)	[26]
	S	[25]
7-(H <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> -8-OH-C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	S	[6]
μ-7,8-(CH <sub>2</sub> ) <sub>4</sub> CHB(OMe) <sub>2</sub> -7-CB <sub>10</sub> H <sub>11</sub> <sup>-</sup>	S, X, H, B, C	[577]
μ-7,8-(CH <sub>2</sub> ) <sub>4</sub> CHOH-7-CB <sub>10</sub> H <sub>11</sub> <sup>-</sup>	S, X, H, B, C	[577]
7-[PhC(O)NH]CB <sub>10</sub> H <sub>11</sub> -SMe <sub>2</sub>	S, UV, IR	[6]
7-(Me <sub>3</sub> Si) <sub>2</sub> CH-7-CB <sub>10</sub> H <sub>11</sub> -9-SMe <sub>2</sub>	S, H, B, MS, IR	[15]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> -2, 4-C <sub>6</sub> H <sub>3</sub> S(NO <sub>2</sub> ) <sub>2</sub>	S	[29]
7-(RNH)CB <sub>10</sub> H <sub>10</sub> -2-SMe <sub>2</sub> -11-Me <sub>3</sub> SiR'C=CH R=PhCH <sub>2</sub> , CMe <sub>3</sub> , Bu; R'=SiMe <sub>3</sub> , Bu	S, H, B, MS	[3]
7-CB <sub>10</sub> H <sub>12</sub> -8-SMe <sub>2</sub>	S, H, B, IR, MS	[27]
(2)-1-[(Me <sub>3</sub> C)HN]CB <sub>10</sub> H <sub>10</sub> -3-C <sub>6</sub> H <sub>11</sub> -5-SMe <sub>2</sub>	S, X, H, B, MS, IR	[4]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> Cl	S, IR, MS	[5]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>6</sub> D <sub>5</sub> -9-Cl	S, H, B (2d), MS, IR	[22]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> - <i>n</i> -Cl, <i>n</i> =4, 9	S, H, B(2d), MS	[21]
<i>Anti</i> -9-(Me <sub>3</sub> CNH <sub>2</sub> )CB <sub>10</sub> H <sub>10</sub> - <i>conjuncto</i> -B <sub>8</sub> H <sub>10</sub>	S, X, H, B, MS	[292]
<b>Detailed NMR Studies</b>		
μ-PhCH-PhCB <sub>10</sub> H <sub>11</sub> <sup>-</sup> (1,2; 1,7)	C	[294]
μ-MeCH-MeCB <sub>10</sub> H <sub>11</sub> <sup>-</sup> (1,2; 1,7)	C	[294]
<b>Other Experimental Studies</b>		
[BH <sub>2</sub> (NMe <sub>3</sub> ) <sub>2</sub> <sup>+</sup> ] [7-CB <sub>10</sub> H <sub>13</sub> <sup>-</sup> ]	Thermal decomposition	
[-(CH <sub>2</sub> ) <sub><i>n</i></sub> -NH(CB <sub>10</sub> H <sub>12</sub> ) <sup>-</sup> ] <sub><i>n</i></sub> polymers	Copolymerization of CB <sub>10</sub> H <sub>12</sub> <sup>-</sup> anion with dibromoalkanes, crosslinking with Co <sup>3+</sup>	[43]
7-CB <sub>10</sub> H <sub>13</sub> <sup>-</sup> , 7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>12</sub>	Controlled chemical and electrochemical substitution [Cl, D, OH, CO, C(O)OH]	[21]
<b>Theoretical Studies</b>		
<b>Molecular and electronic structure calculations</b>		
7-CB <sub>10</sub> H <sub>12</sub> -8-OH <sup>-</sup>	Δ <i>H<sub>f</sub></i> , IP, charge distribution, bond indices	[21]
7-(H <sub>2</sub> N)CB <sub>10</sub> H <sub>11</sub> -4-Cl <sup>-</sup>	Δ <i>H<sub>f</sub></i> , IP, charge distribution, bond indices	[21]
7-(H <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> - <i>n</i> -Cl, <i>n</i> =4,9	Δ <i>H<sub>f</sub></i> , IP, charge distribution, bond indices	[21]
7-(H <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> - <i>n</i> -OH, <i>n</i> =8,9	Δ <i>H<sub>f</sub></i> , IP, charge distribution, bond indices	[21]
7-(H <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> -8-NH <sub>3</sub>	Δ <i>H<sub>f</sub></i> , IP, charge distribution, bond indices	[21]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>12</sub>	Δ <i>H<sub>f</sub></i> , IP, charge distribution, bond indices	[21]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> -4-Ph-CH <sub>2</sub> =CHCH <sub>2</sub>	Δ <i>H<sub>f</sub></i> , charge distribution	[23]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>11</sub> -4-X, X=I, Br	Δ <i>H<sub>f</sub></i> , charge distribution	[23]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>10</sub> -4,6-X <sub>2</sub> , X=I, Br	Δ <i>H<sub>f</sub></i> , charge distribution	[23]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>9</sub> -4-I <sub>2</sub> <sup>-</sup>	Δ <i>H<sub>f</sub></i> , charge distribution	[23]
7-(Me <sub>3</sub> N)CB <sub>10</sub> H <sub>8</sub> -4,6-I <sub>2</sub> <sup>2-</sup>	Δ <i>H<sub>f</sub></i> , charge distribution	[23]

Compound	Information	References
<i>NMR calculations</i>		
7-CB <sub>10</sub> H <sub>10</sub> -μ(9,10)-CHMe <sup>-</sup>	GIAO ( <sup>11</sup> B)	[296]
<i>Reactivity calculations</i>		
7-CB <sub>10</sub> H <sub>10</sub> -μ(9,10)-CHMe <sup>-</sup>	pK <sub>a</sub>	[296]
<sup>a</sup> S, synthesis; X, X-ray diffraction; H, <sup>1</sup> H NMR; B, <sup>11</sup> B NMR; C, <sup>13</sup> C NMR; 2d, two-dimensional (COSY) NMR; IR, infrared data; MS, mass spectroscopic data; UV, UV-visible data; E, electrochemical data; IP, ionization potential.		