

Thermodynamic Hydrlicity of Small Borane Clusters and Polyhedral *closo*-Boranes [†]

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[†] Dedicated to Professor Bohumil Štibr (1940-2020), who unfortunately passed away before he could reach the age of 80, in the recognition of his outstanding contributions to boron chemistry.

Supplementary Materials

- Scheme S1.** Scheme of homologous series of neutral and monoanionic boranes clusters. **S3**
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- Scheme S3.** $\text{Li}_2[\text{B}_n\text{H}_{3n}]$ series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets is difference in Gibbs energy ($\Delta G^{\circ}_{\text{MeCN}}$ in kcal/mol) relative to the most stable isomer. Lithium atoms are omitted for clarity. **S6**
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- Scheme S5.** $\text{B}_n\text{H}_{3n-2}$ series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets is difference in Gibbs energy ($\Delta G^{\circ}_{\text{MeCN}}$ in kcal/mol) relative to the most stable isomer. **S8**

Table S6. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for $\text{B}_n\text{H}_{3n-2}$ series. **S8**

Scheme S6. $\text{Li}_2[\text{B}_n\text{H}_{3n-2}]$ series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets is difference in Gibbs energy ($\Delta G^{\circ}_{\text{MeCN}}$ in kcal/mol) relative to the most stable isomer. Lithium atoms are omitted for clarity. **S9**

Table S7. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for $\text{Li}_2[\text{B}_n\text{H}_{3n-2}]$ series. **S10**

Scheme S7. $\text{Li}[\text{B}_n\text{H}_{3n-3}]$ series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets is difference in Gibbs energy ($\Delta G^{\circ}_{\text{MeCN}}$ in kcal/mol) relative to the most stable isomer. Lithium atoms are omitted for clarity. **S11**

Table S8. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for $\text{Li}[\text{B}_n\text{H}_{3n-3}]$ series. **S12**

Scheme S8. $\text{B}_n\text{H}_{3n-4}$ series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets is difference in Gibbs energy ($\Delta G^{\circ}_{\text{MeCN}}$ in kcal/mol) relative to the most stable isomer. **S13**

Table S9. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for $\text{B}_n\text{H}_{3n-4}$ series. **S14**

Structural features of polyhedral closo-boranes **S15**

Figure S2. NPA charge distribution (showed in blue-green-red scale from -0.40 to 0.05), calculated for M06-optimized geometries of dianions $[\text{B}_n\text{H}_n]^{2-}$ ($n = 5-17$) of polyhedral closo-boranes in MeCN. **S16**

Table S10. Coordination numbers (CN) of boron atom in polyhedral closo-boranes. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol). **S17**

Table S11. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol). **S18**

Figure S3. HDA^{MeCN} of polyhedral closo-boranes $\text{Li}_2[\text{B}_n\text{H}_n]$ ($n = 5-17$). Blue columns represent lowest HDA^{MeCN} values, red columns – highest. **S19**

Scheme S9. General trend of HDA^{MeCN} for $\text{Li}_2[\text{B}_n\text{H}_n]$ ($n = 2-4$). **S19**

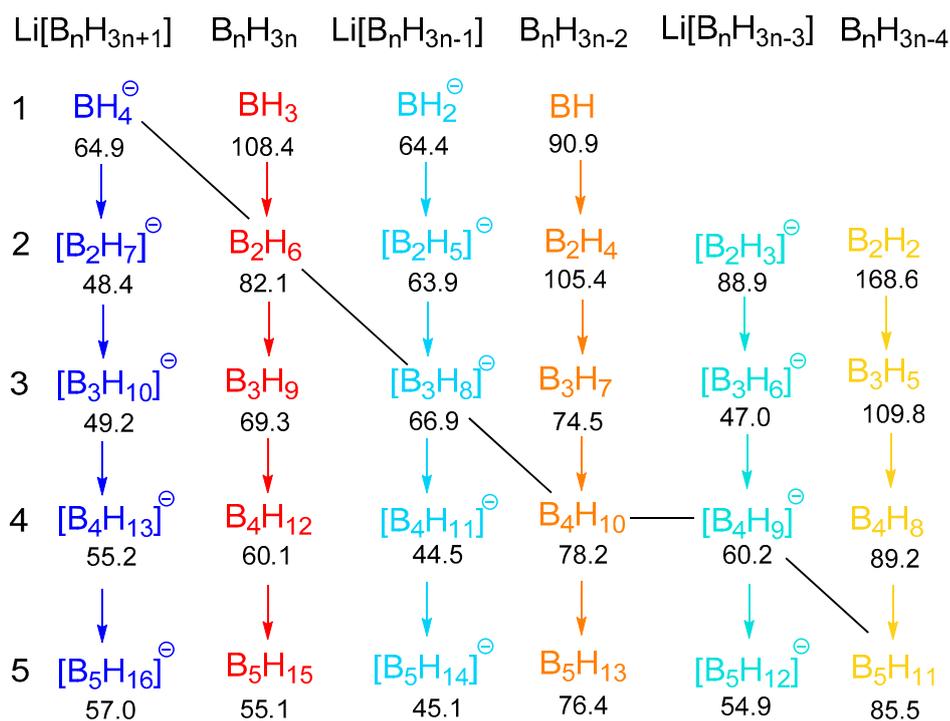
Scheme S10. General trend of HDA^{MeCN} for polyhedral closo-boranes $\text{Li}_2[\text{B}_n\text{H}_n]$ ($n = 5-17$). **S19**

Figure S4. Plot HDA^{MeCN} vs bond length of terminal B–H bond for Li salts polyhedral closo-boranes (green triangles), neutral and anionic borane clusters (red circles) and tetracoordinated boron hydrides (blue squares). HDA^{MeCN} for tetracoordinated boron hydrides are taken from ref.[5] **S20**

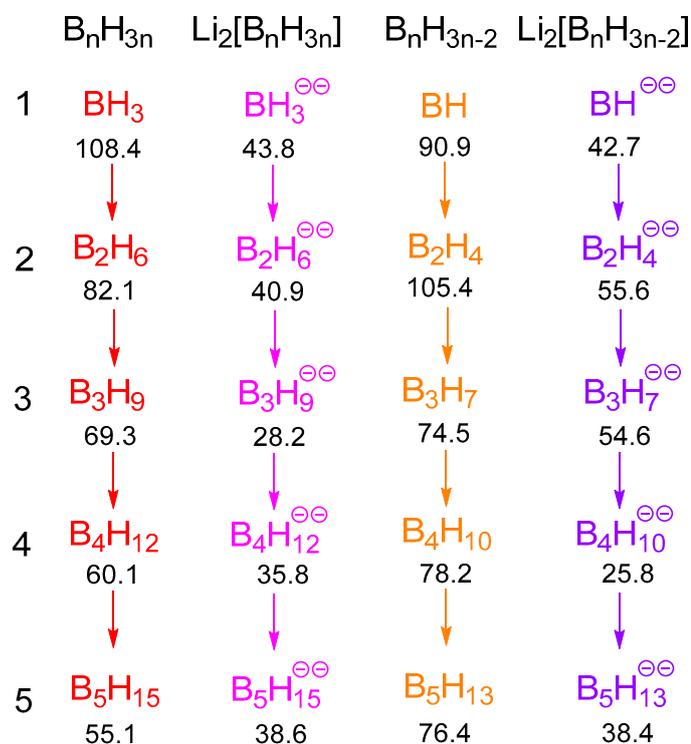
Figure S5. Free Gibbs energy per BH unit calculated for dianions $[\text{B}_n\text{H}_n]^{2-}$ ($n = 5-17$) of polyhedral closo-boranes and their Li-salts $\text{Li}_2[\text{B}_n\text{H}_n]$ in ($n = 5-17$) MeCN vs number boron atoms. **S21**

Figure S6. Graph of normalized lowest HDA^{MeCN} of and free Gibbs energy per BH unit for dianions $[\text{B}_n\text{H}_n]^{2-}$ ($n = 5-17$) of polyhedral closo-boranes vs number boron atoms. **S21**

Table S12. DFT-optimized geometries (Cartesian coordinates) and electronic energies **S22–S42**



Scheme S1. Scheme of homologous series of neutral and monoanionic boranes clusters. The values of HDA^{MeCN} are given in black for the most energetically favorable isomer. Lithium atoms are omitted for clarity.



Scheme S2. Homologous series of neutral and dianionic boranes clusters. The values of HDA^{MeCN} are given in black for the most energetically favorable isomer. Lithium atoms are omitted for clarity.

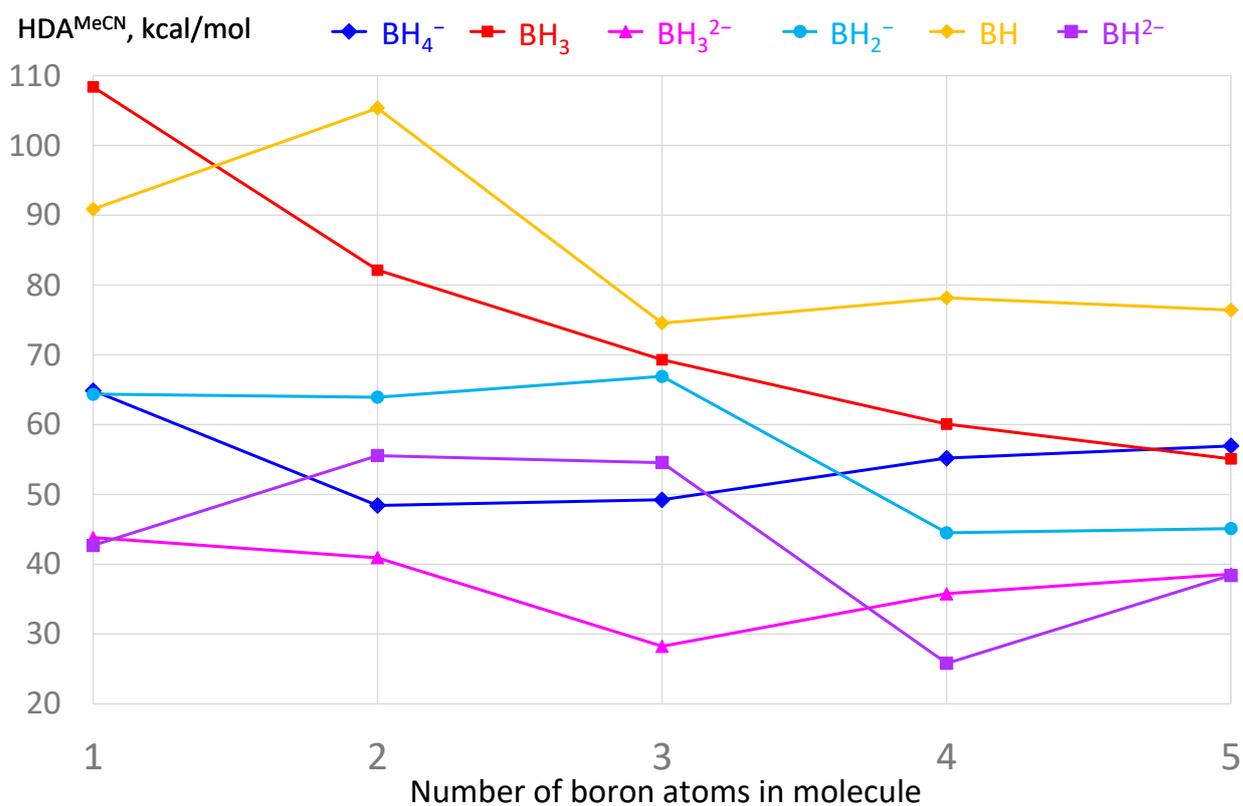


Figure S1. Plots of HDA^{MeCN} against the number of boron atoms in borane clusters derived from different starting species.

Table S1. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for $\text{Li}[\text{B}_n\text{H}_{3n+1}]$ series.

Borohydride	$\Delta G^{\circ}_{\text{MeCN}}$	$r(\text{B-H})$	HDA^{MeCN}	$\Delta H^{\circ}_{[\text{H}]^-\text{MeCN}}$
LiBH₄	—	1.206	64.86	72.77
Li[B₂H₇]	—	1.214	48.42	54.96
Li[B₃H₁₀]	—	1.210	49.22	55.54
<i>n</i> -Li[B ₄ H ₁₃]	0.0	1.206	55.20	62.13
<i>i</i> -Li[B ₄ H ₁₃]	5.2	1.207	55.65	61.78
<i>n</i> -Li[B ₅ H ₁₆]	0.0	1.204	56.95	62.61
<i>i</i> -Li[B ₅ H ₁₆]	5.9	1.212	59.36	66.05
<i>t</i> -Li[B ₅ H ₁₆]	13.5	1.208	48.96	54.29

n – normal, *i* – isomeric, *t* – tertiary.

Table S2. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for B_nH_{3n} series.

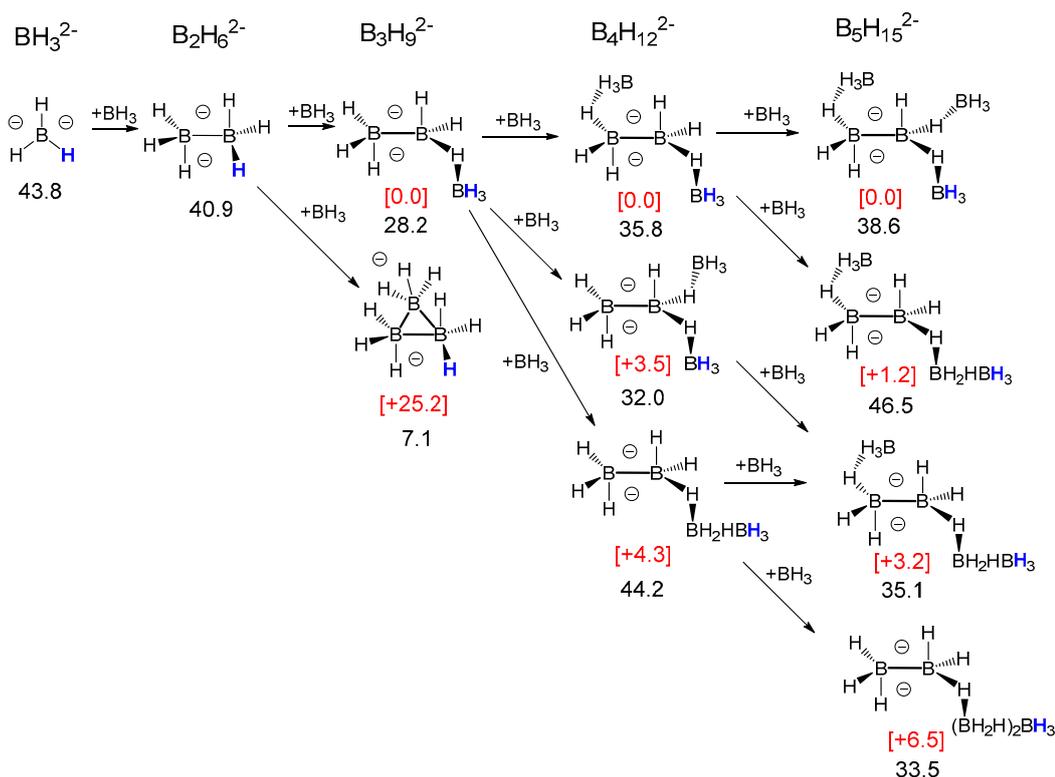
Borohydride	$\Delta G^\circ_{\text{MeCN}}$	r(B–H)	HDA ^{MeCN}	$\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$
BH₃	–	1.186	108.38	114.43
B₂H₆	–	1.186	82.12	89.19
<i>lin</i> -B ₃ H ₉	0.0	1.202	69.32	75.69
<i>btf</i> -B ₃ H ₉	0.5	1.190	68.51	75.75
<i>cyc</i> -B ₃ H ₉	2.3	1.193	72.62	79.54
<i>lin</i> -B ₄ H ₁₂	0.0	1.204	60.08	66.17
<i>pinc</i> -B ₄ H ₁₂	4.5	1.200	55.36	60.16
<i>cyc</i> -B ₄ H ₁₂	9.5	1.193	65.13	71.45
<i>lin</i> -B ₅ H ₁₅	0.0	1.202	55.09	60.85
<i>i</i> -B ₅ H ₁₅	3.9	1.200	62.40	70.67
<i>pinc</i> -B ₅ H ₁₅	7.1	1.203	59.10	66.07
<i>cyc</i> -B ₅ H ₁₅	8.1	1.197	65.35	72.10

lin – linear, *btf* – butterfly-like, *cyc* – cyclic, *pinc* – pincer-like, *i* – isomeric.

Table S3. Difference in Gibbs energy ($\Delta G^\circ_{\text{MeCN}}$ in kcal/mol) relative to the most stable isomer of B₃H₉ in MeCN ($\Delta G^\circ_{\text{MeCN}}$ in kcal/mol), B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol).

MP2/6-311++G(d,p)	$\Delta G^\circ_{\text{MeCN}}$	r(B–H)	HDA ^{MeCN}	$\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$
B₂H₅(μ-H)BH₃ (<i>lin</i>-B₃H₉)	0.0	1.203	72.18	78.50
<i>btf</i> -B ₃ H ₉	0.8	1.191	71.33	78.63
<i>cyc</i> -B ₃ H ₉	1.3	1.191	76.61	83.42
M06/6-311++G(d,p)	$\Delta G^\circ_{\text{MeCN}}$	r(B–H)	HDA ^{MeCN}	$\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$
B₂H₅(μ-H)BH₃ (<i>lin</i>-B₃H₉)	0.0	1.202	69.32	75.69
<i>btf</i> -B ₃ H ₉	0.5	1.190	68.51	75.75
<i>cyc</i> -B ₃ H ₉	2.3	1.193	72.62	79.54

lin – linear, *btf* – butterfly-like, *cyc* – cyclic.

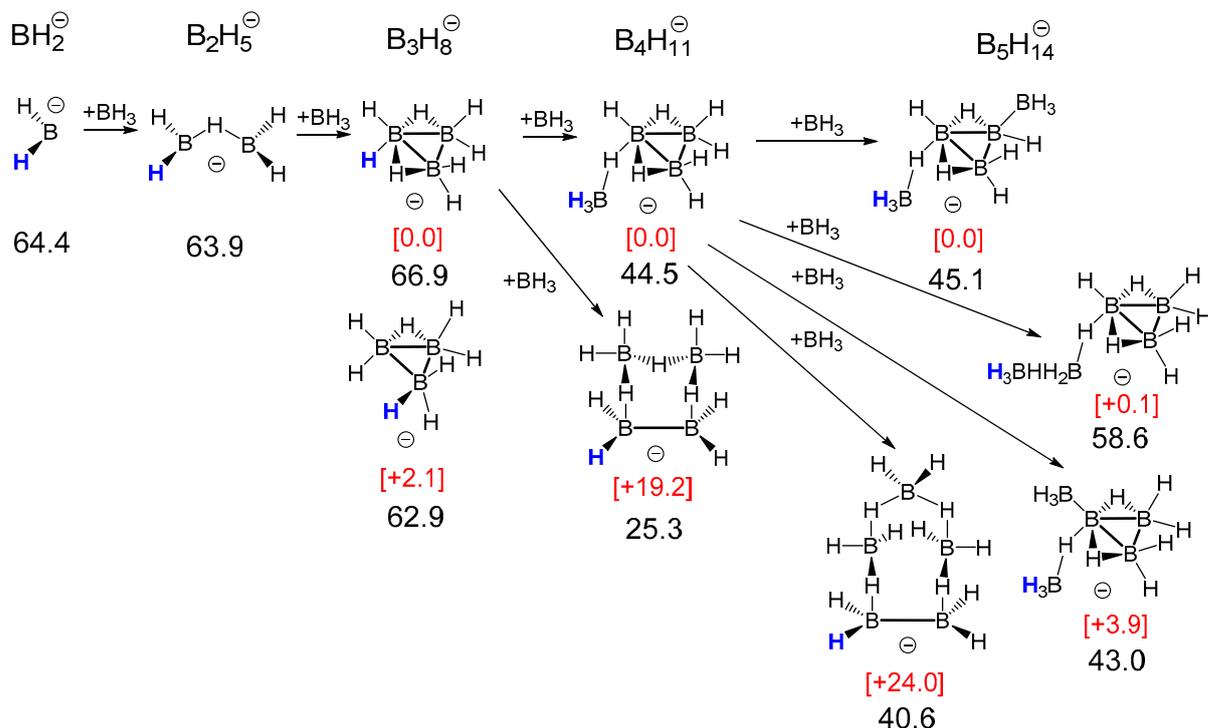


Scheme S3. Li₂[B_nH_{3n}] series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets indicate difference in Gibbs energy (ΔG^{MeCN} in kcal/mol) relative to the most stable isomer. Lithium atoms are omitted for clarity.

Table S4. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^{\circ}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for Li₂[B_nH_{3n}] series.

Borohydride	$\Delta G^{\circ}_{\text{MeCN}}$	r(B–H)	HDA ^{MeCN}	$\Delta H^{\circ}_{[\text{H}]^-\text{MeCN}}$
Li ₂ BH ₃	—	1.237	43.82	52.34
Li ₂ [B ₂ H ₆]	—	1.241	40.94	48.55
<i>lin</i> -Li ₂ [B ₃ H ₉]	0.0	1.248	28.24	35.02
<i>cyc</i> -Li ₂ [B ₃ H ₉]	25.2	1.227	7.05	14.56
<i>1,2</i> -Li ₂ [B ₄ H ₁₂]	0.0	1.236	35.78	42.71
<i>1,1</i> -Li ₂ [B ₄ H ₁₂]	3.5	1.229	32.04	38.24
<i>lin</i> -Li ₂ [B ₄ H ₁₂]	4.3	1.233	44.16	51.41
<i>pinc</i> -Li ₂ [B ₅ H ₁₂]	0.0	1.218	38.55	44.71
<i>1,2</i> -Li ₂ [B ₅ H ₁₂]	1.2	1.228	46.53	53.50
<i>1,1</i> -Li ₂ [B ₅ H ₁₂]	3.2	1.235	35.05	40.50
<i>lin</i> -Li ₂ [B ₅ H ₁₂]	6.5	1.253	33.54	39.92

lin – linear, *cyc* – cyclic, *pinc* – pincer-like.

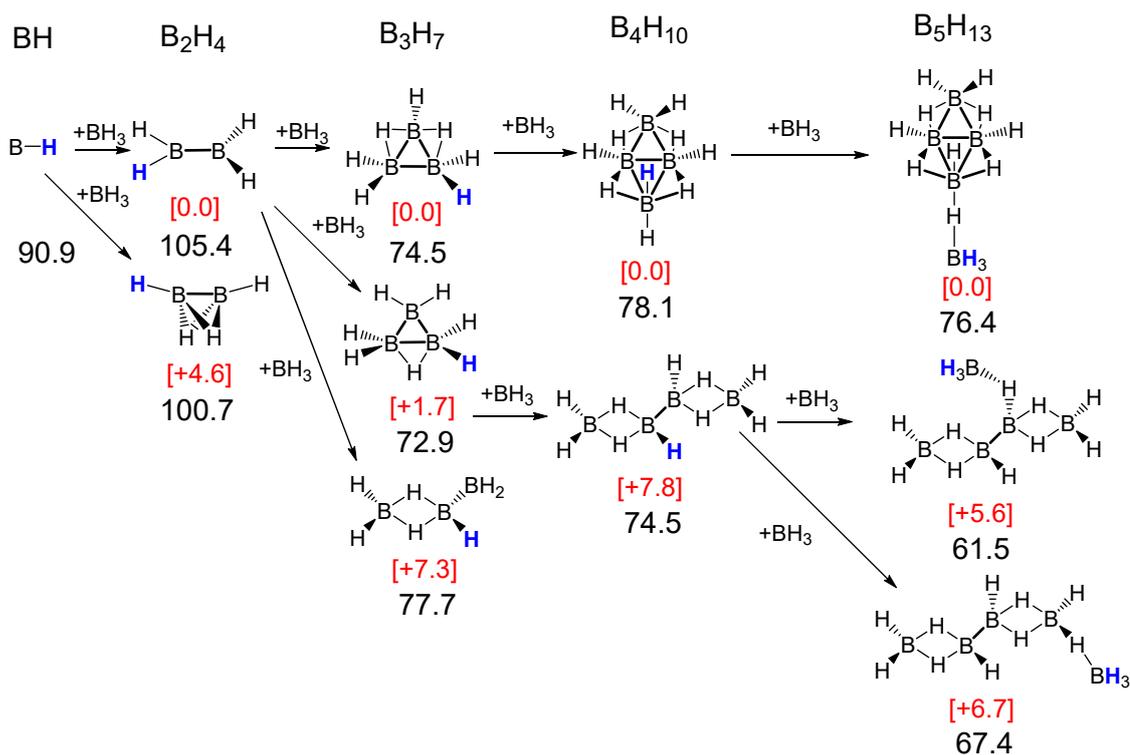


Scheme S4. $\text{Li}[\text{B}_n\text{H}_{3n-1}]$ series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets is difference in Gibbs energy (ΔG^{MeCN} in kcal/mol) relative to the most stable isomer. Lithium atoms are omitted for clarity.

Table S5. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\text{MeCN}}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^{\text{MeCN}}_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for $\text{Li}[\text{B}_n\text{H}_{3n-1}]$ series.

Borohydride	ΔG^{MeCN}	r(B–H)	HDA^{MeCN}	$\Delta H^{\text{MeCN}}_{[\text{H}]^-\text{MeCN}}$
LiBH_2	–	1.220	64.36	66.64
$\text{Li}[\text{B}_2\text{H}_5]$	–	1.217	63.94	71.81
$\text{Li}[\text{B}_3\text{H}_8]$ conf0	0.0	1.208	66.91	74.65
$\text{Li}[\text{B}_3\text{H}_8]$ conf1	2.1	1.222	62.85	70.95
<i>lin</i> - $\text{Li}[\text{B}_4\text{H}_{11}]$	0.0	1.208	44.50	51.54
<i>cyc</i> - $\text{Li}[\text{B}_4\text{H}_{11}]$	19.2	1.227	25.27	32.48
<i>1,2</i> - $\text{Li}[\text{B}_5\text{H}_{14}]$	0.0	1.204	45.11	51.04
<i>lin</i> - $\text{Li}[\text{B}_5\text{H}_{14}]$	0.1	1.207	58.64	65.88
<i>1,1</i> - $\text{Li}[\text{B}_5\text{H}_{14}]$	3.9	1.205	43.03	48.81
<i>cyc</i> - $\text{Li}[\text{B}_5\text{H}_{14}]$	24.0	1.228	40.60	45.51

lin – linear, cyc – cyclic.

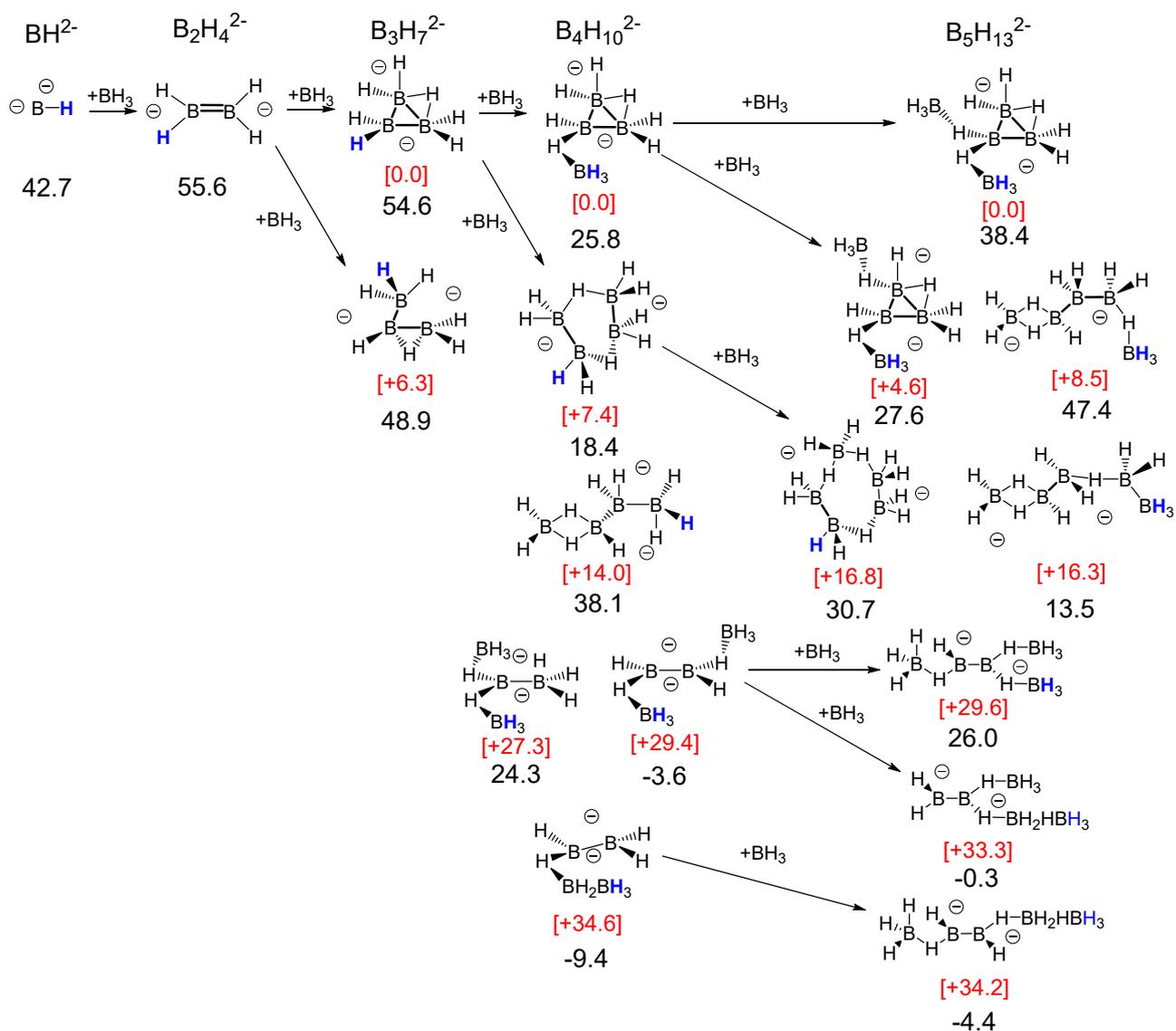


Scheme S5. B_nH_{3n-2} series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets is difference in Gibbs energy (ΔG°_{MeCN} in kcal/mol) relative to the most stable isomer.

Table S6. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^\circ_{[H]^-MeCN}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^\circ_{[H]^-MeCN}$ in kcal/mol) for B_nH_{3n-2} series.

Borohydride	ΔG°_{MeCN}	$r(B-H)$	HDA^{MeCN}	$\Delta H^\circ_{[H]^-MeCN}$
BH	—	1.213	90.88	96.30
<i>st</i> - B_2H_4	0.0	1.194	105.35	112.51
<i>btf</i> - B_2H_4	4.6	1.168	100.72	108.64
$B_3H_5(\mu_2H)_2$ (B_3H_7)	0.0	1.191	74.54	81.52
$B_3H_6(\mu_2H)$ (B_3H_7)	1.7	1.191	72.91	79.67
$B_2H_5(BH_2)$ (B_3H_7)	7.3	1.196	77.65	85.01
<i>arachno</i> - B_4H_{10}	0.0	1.192	78.17	84.97
<i>bis</i> - B_4H_{10}	7.8	1.193	74.52	80.94
<i>arachno</i> - $B_4H_{10}(BH_3)$	0.0	1.197	76.40	81.96
<i>i-bis</i> - $B_4H_{10}(BH_3)$	5.6	1.200	61.46	67.19
<i>n-bis</i> - $B_4H_{10}(BH_3)$	6.4	1.203	67.72	73.79

st – staggered, btf – butterfly-like, n – normal, i – isomeric.

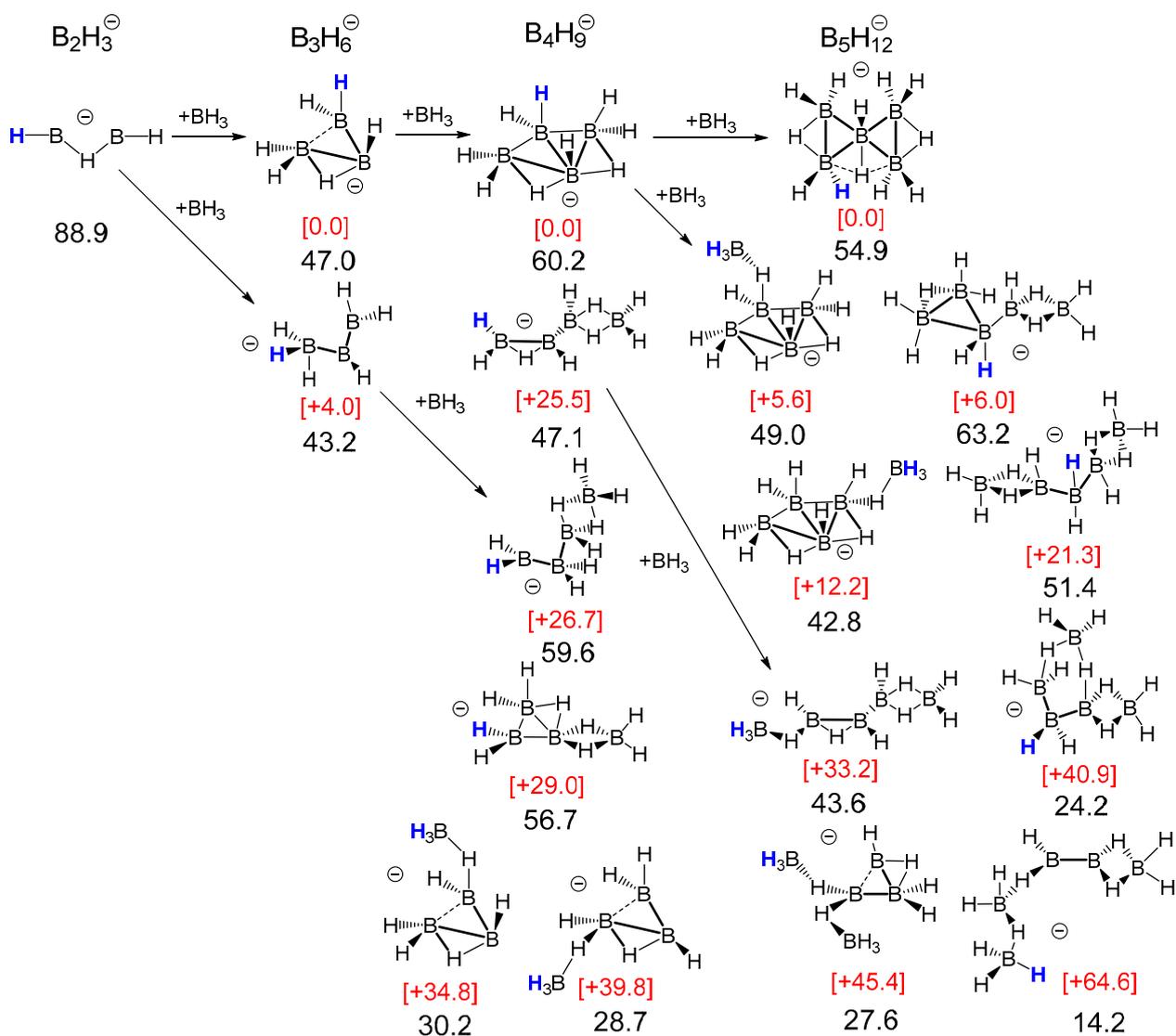


Scheme S6. $\text{Li}_2[\text{B}_n\text{H}_{3n-2}]$ series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets indicate difference in Gibbs energy ($\Delta G^\circ_{\text{MeCN}}$ in kcal/mol) relative to the most stable isomer. Lithium atoms are omitted for clarity.

Table S7. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for Li₂[B_nH_{3n-2}] series.

Borohydride	$\Delta G^\circ_{\text{MeCN}}$	r(B–H)	HDA ^{MeCN}	$\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$
Li ₂ BH	–	1.222	42.70	48.02
Li ₂ [B ₂ H ₄]	–	1.220	55.57	65.00
Li ₂ [B ₃ H ₇] conf0	0.0	1.225	54.56	63.19
Li ₂ [B ₃ H ₇] conf1	6.3	1.238	48.91	57.39
<i>lin</i> -Li ₂ [B ₄ H ₁₀]	0.0	1.227	25.80	32.04
<i>cyc</i> -Li ₂ [B ₄ H ₁₀]	7.4	1.227	18.42	26.16
<i>bis</i> -Li ₂ [B ₄ H ₁₀]	14.0	1.250	38.13	45.35
<i>pinc</i> -BB-Li ₂ [B ₄ H ₁₀]	27.3	1.212	24.28	30.54
<i>tr</i> -BB-Li ₂ [B ₄ H ₁₀]	29.4	1.213	-3.56	2.03
<i>lin</i> -BB-Li ₂ [B ₄ H ₁₀]	34.6	1.219	-9.41	-4.51
<i>1,1</i> -Li ₂ [B ₅ H ₁₃]	0.0	1.215	38.41	46.30
<i>1,2</i> -Li ₂ [B ₅ H ₁₃]	4.6	1.217	27.61	34.17
<i>bis</i> -Li ₂ [B ₅ H ₁₃] conf0	8.5	1.244	47.43	54.18
<i>bis</i> -Li ₂ [B ₅ H ₁₃] conf1	16.3	1.249	13.54	18.93
<i>cyc</i> -Li ₂ [B ₅ H ₁₃]	16.8	1.235	30.71	36.27
<i>pinc</i> -BB-Li ₂ [B ₅ H ₁₃]	29.6	1.213	26.03	32.09
<i>1,1</i> -BB-Li ₂ [B ₅ H ₁₃]	33.3	1.212	-0.27	4.59
<i>tr</i> -BB-Li ₂ [B ₅ H ₁₃]	34.2	1.212	-4.38	0.96

lin – linear, *cyc* – cyclic, *pinc* – pincer-like, *tr* – trans.

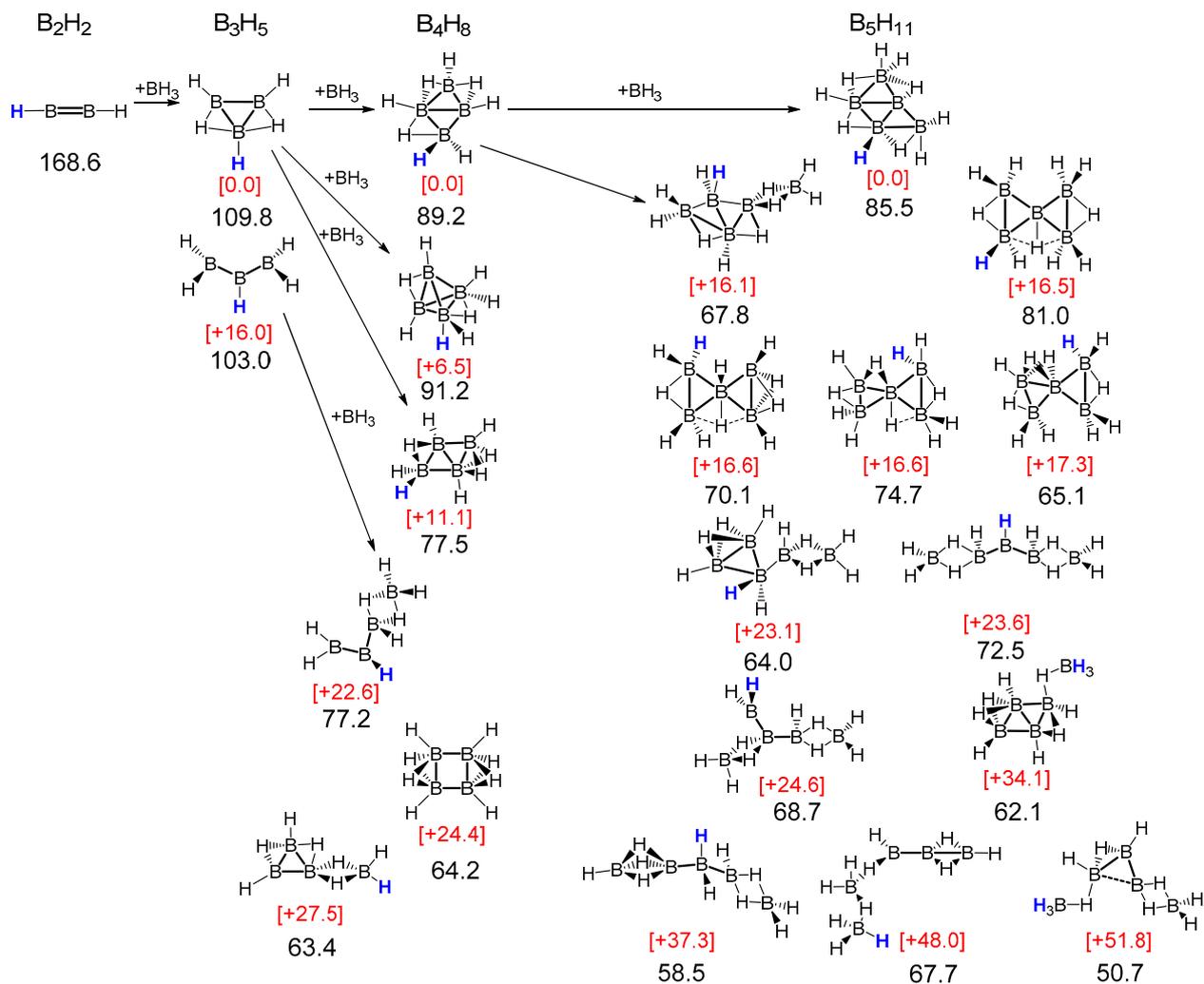


Scheme S7. $Li[B_nH_{3n-3}]$ series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets is difference in Gibbs energy (ΔG^{MeCN} in kcal/mol) relative to the most stable isomer. Lithium atoms are omitted for clarity.

Table S8. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for Li[B_nH_{3n-3}] series.

Borohydride	$\Delta G^\circ_{\text{MeCN}}$	r(B–H)	HDA ^{MeCN}	$\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$
Li[B ₂ H ₃]	–	1.178	88.90	96.60
Li[B ₃ H ₆] conf0	0.0	1.220	47.01	54.75
Li[B ₃ H ₆] conf1	4.0	1.232	43.15	50.42
<i>arachno</i> -Li[B ₄ H ₉]	0.0	1.210	60.19	68.19
<i>bis</i> -Li[B ₄ H ₉] conf0	25.5	1.221	47.09	53.49
<i>bis</i> -Li[B ₄ H ₉] conf1	26.7	1.224	59.63	67.94
<i>lin</i> - <i>BBB</i> -Li[B ₄ H ₉] conf0	29.0	1.224	56.68	64.22
<i>lin</i> -1- <i>BBB</i> -Li[B ₄ H ₉] conf1	34.8	1.215	30.18	35.69
<i>lin</i> -3- <i>BBB</i> -Li[B ₄ H ₉] conf1	39.8	1.209	28.70	35.30
<i>commo</i> -Li[B ₅ H ₁₂]	0.0	1.205	54.90	61.86
<i>lin</i> -1-Li[B ₅ H ₁₂]	5.6	1.212	49.04	55.33
<i>lin</i> - <i>BBB</i> -Li[B ₅ H ₁₂]	6.0	1.223	63.20	71.16
<i>lin</i> -2-Li[B ₅ H ₁₂]	12.2	1.214	42.77	49.06
<i>bis</i> - <i>BH</i> ₂ -Li[B ₅ H ₁₂]	21.3	1.240	51.41	58.82
<i>lin</i> - <i>bis</i> -Li[B ₅ H ₁₂]	33.2	1.212	43.63	51.55
<i>lin</i> - <i>cyc</i> -Li[B ₅ H ₁₂]	40.9	1.234	24.20	30.99
1,1- <i>BBB</i> -Li[B ₅ H ₁₂]	45.4	1.213	11.20	15.49
<i>lin</i> - <i>BB</i> -Li[B ₅ H ₁₂]	64.6	1.212	14.19	20.89

lin – linear, *cyc* – cyclic.



Scheme S8. B_nH_{3n-4} series. Black numbers denote HDA^{MeCN} (in kcal/mol), red numbers in square brackets is difference in Gibbs energy (ΔG^{MeCN} in kcal/mol) relative to the most stable isomer.

Table S9. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) for B_nH_{3n-4} series.

Borohydride	$\Delta G^\circ_{\text{MeCN}}$	r(B–H)	HDA ^{MeCN}	$\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$
B₂H₂	—	1.168	168.58	178.45
B₃H₅ conf0	0.0	1.173	109.84	117.88
B₃H₅ conf1	16.0	1.202	103.05	110.27
<i>arachno</i> -B ₄ H ₈ conf0	0.0	1.195	89.24	96.90
<i>disph</i> -B ₄ H ₈	6.5	1.191	91.15	98.01
<i>arachno</i> -B ₄ H ₈ conf1	11.1	1.198	77.54	85.03
<i>bis</i> -B ₄ H ₈	22.6	1.200	77.17	84.45
<i>sq</i> -B ₄ H ₈	24.4	1.192	64.24	72.13
<i>lin</i> -BBB-B ₄ H ₈	27.5	1.187	63.37	70.63
<i>arachno</i> -B ₅ H ₁₁	0.0	1.195	85.52	93.14
<i>lin</i> -1-B ₅ H ₁₁ conf0	16.1	1.199	67.79	74.57
<i>commo</i> -B ₅ H ₁₁ conf0	16.5	1.193	81.04	87.76
<i>commo</i> -B ₅ H ₁₁ conf1	16.6	1.199	70.09	77.60
<i>commo</i> -B ₅ H ₁₁ conf2	16.6	1.195	74.73	82.65
<i>commo</i> -B ₅ H ₁₁ conf3	17.3	1.194	65.12	70.89
<i>lin</i> -BBB-B ₅ H ₁₁ conf0	23.1	1.212	63.97	70.32
<i>bis</i> -BH-B ₅ H ₁₁	23.6	1.199	72.54	77.61
<i>i-bis</i> -B ₄ H ₈ (BH ₃)	24.6	1.194	68.67	74.20
<i>lin</i> -1-B ₅ H ₁₁ conf1	34.1	1.199	62.11	68.27
<i>bis</i> -BH ₂ -B ₅ H ₁₁	37.3	1.223	58.51	65.07
<i>lin</i> -BB-B ₅ H ₁₁	48.0	1.201	67.76	74.55
1,2-BBB-LiB₅H₁₁ conf1	51.8	1.200	50.67	57.16

disp – disphenoidal, *lin* – linear, *sq* – squared, *i* – isomeric.

Structural features of polyhedral closo-boranes

From $[\text{B}_5\text{H}_5]^{2-}$ to $[\text{B}_7\text{H}_7]^{2-}$ a bent of polyhedron represent triangle, square and pentagon, however $[\text{B}_6\text{H}_6]^{2-}$ have geometry of octahedron with equivalent B–H vertices. In the structure of $[\text{B}_8\text{H}_8]^{2-}$ consist two caps formed of B_2H_2 fragments and B_4H_4 hyper shaped structure in the heart of the polyhedron belt which is a transitional form between planar and 3D structure patterns forming bent of polyhedron of closo-boranes.

In the next structures bent of polyhedron has shape of trigonal prism for $[\text{B}_9\text{H}_9]^{2-}$, tetragonal antiprism for $[\text{B}_{10}\text{H}_{10}]^{2-}$, pentagonal antiprism for $[\text{B}_{12}\text{H}_{12}]^{2-}$, hexagonal antiprism for $[\text{B}_{14}\text{H}_{14}]^{2-}$. $[\text{B}_{12}\text{H}_{12}]^{2-}$ is icosahedron with equivalent B–H vertices, however it neighbors of octadecahedral $[\text{B}_{11}\text{H}_{11}]^{2-}$ and docosahedral $[\text{B}_{13}\text{H}_{13}]^{2-}$ having a low symmetry C_{2v} . Polyhedron bent in their structures consists of two molecular subunits, which combined basket-shape and bowl-shape structures, correspondingly. In the next three closo-boranes an evolution of capping structures is observed: triangles in $[\text{B}_{15}\text{H}_{15}]^{2-}$, squares in $[\text{B}_{16}\text{H}_{16}]^{2-}$ and pentagonal pyramids in $[\text{B}_{17}\text{H}_{17}]^{2-}$. At the same involution of polyhedron bent takes places: hexagonal rhombus loop, contained two types atoms of different reactivity in $[\text{B}_{15}\text{H}_{15}]^{2-}$, antiprismatic octagon in $[\text{B}_{16}\text{H}_{16}]^{2-}$ and expanded pentagonal ring in $[\text{B}_{17}\text{H}_{17}]^{2-}$. In this way $[\text{B}_{17}\text{H}_{17}]^{2-}$ formally can be formed by breaking icosahedral structure of $[\text{B}_{12}\text{H}_{12}]^{2-}$ into two nido- B_6H_6 fragments and insertion B_5H_5 pentagonal ring between them [1].

Natural population analysis (Figure S2) showed that electron density concentrates on boron atoms forming skeleton of polyhedron, whereas hydrogen atoms are less negatively charged. Increasing of BH group involved in polyhedron formation causes repolarization of hydrogens in closo-boranes that apparently explains better hydrolytic stability of large polyhedral closo-boranes [2-4]. In $[\text{B}_n\text{H}_n]^{2-}$ ($n = 5-8$) hydrogens atoms have partial negative charge ($-0.047 \div -0.010$), in $[\text{B}_9\text{H}_9]^{2-}$ the close to zero ($0.001-0.006$), whereas in $[\text{B}_n\text{H}_n]^{2-}$ ($n = 10-17$) the partial positive charge on H is observed ($0.010-0.051$). Terminal B–H groups attached to the most negative charged boron atoms has the shortest bond length. It worth to note that the majority closo-boranes difference between shortest and longest BH bond are $0.04-0.08 \text{ \AA}$ (Figure 4).

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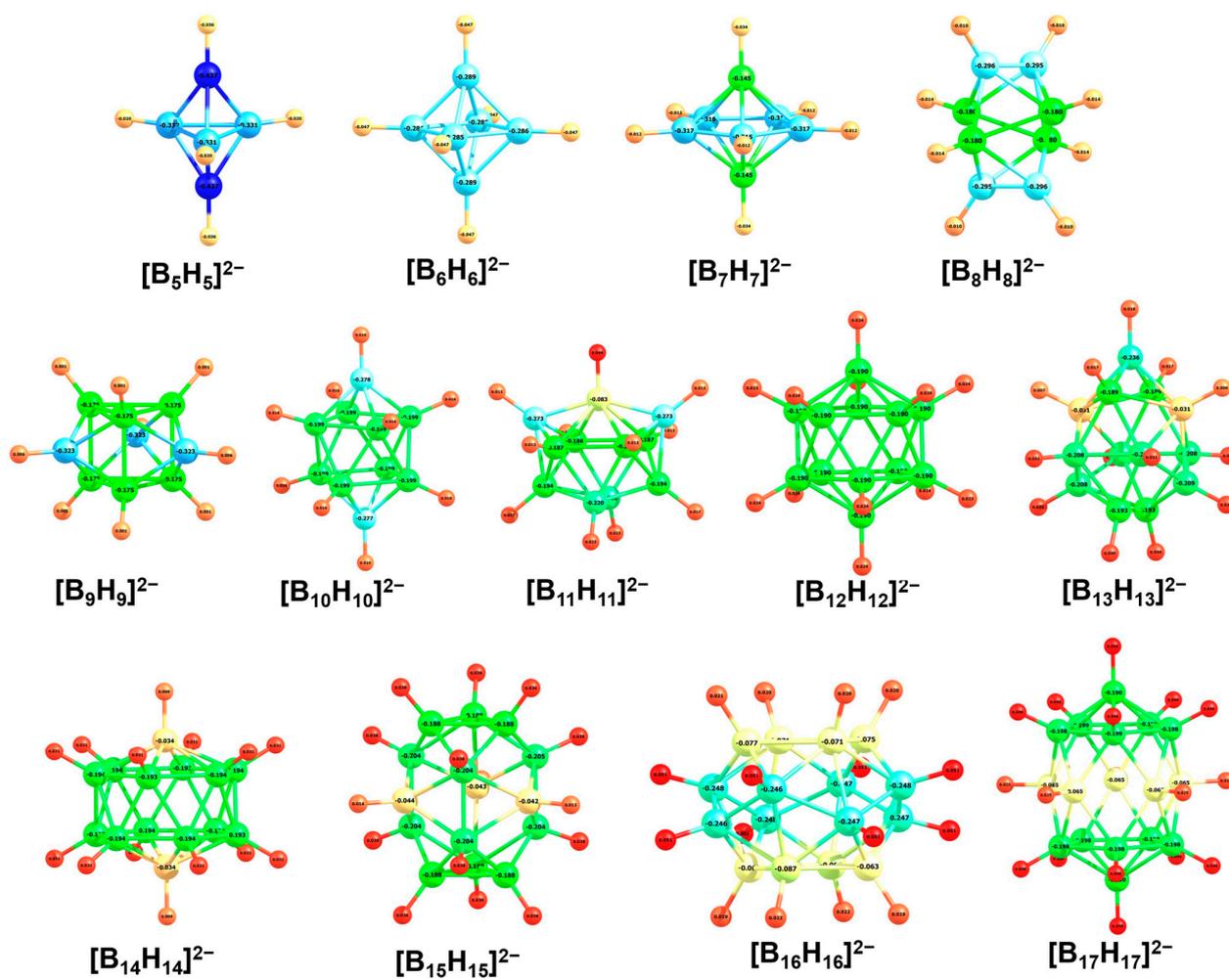


Figure S2. NPA charge distribution (showed in blue-green-red scale from -0.40 to 0.05), calculated for M06-optimized geometries of dianions $[B_nH_n]^{2-}$ (n = 5–17) of polyhedral closo-boranes in MeCN.

Table S10. Coordination numbers (CN) of boron atom in polyhedral closo-boranes. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^{\circ}_{[H]^{-}MeCN}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^{\circ}_{[H]^{-}MeCN}$ in kcal/mol).

Borane	CN(B ^{ap})	CN(B ^{eq})	r(BH ^{ap})	r(BH ^{eq})	HDA ^{MeCN} (BH ^{ap})	$\Delta H^{\circ}_{[H]^{-}MeCN}$ (BH ^{ap})	HDA ^{MeCN} (BH ^{eq})	$\Delta H^{\circ}_{[H]^{-}MeCN}$ (BH ^{eq})
[B ₅ H ₅] ²⁻	4	5	1.194	1.202	81.98	90.31	60.02	68.08
[B ₆ H ₆] ²⁻	5		1.200		71.94	80.07	–	–
[B ₇ H ₇] ²⁻	6	5	1.205	1.199	56.26	64.07	67.58	75.59
[B ₈ H ₈] ²⁻	5	6	1.197	1.203	71.91	80.09	56.79	64.42
[B ₉ H ₉] ²⁻	5	6	1.193	1.199	76.19	84.13	70.82	78.90
[B ₁₀ H ₁₀] ²⁻	5	6	1.191	1.197	89.01	97.05	75.55	83.51
[B ₁₁ H ₁₁] ²⁻	7	5/6	1.199	1.197 1.191	74.50	82.40	65.25 65.32	72.88 72.94
[B ₁₂ H ₁₂] ²⁻	6		1.195		79.60	87.52	–	–
[B ₁₃ H ₁₃] ²⁻	5	5/6	1.192	1.200 1.195 1.198 1.194	39.49	47.76	39.41 39.55 71.41 80.07	47.69 47.80 79.98 88.64
[B ₁₄ H ₁₄] ²⁻	7	6	1.195	1.194	78.99	86.88	75.85	83.79
[B ₁₅ H ₁₅] ²⁻	5	5/6	1.192	1.195 1.194	83.82	91.90	75.28 70.76	83.15 78.90
[B ₁₆ H ₁₆] ²⁻	6	6	1.194	1.192	74.05	82.04	76.86	84.58
[B ₁₇ H ₁₇] ²⁻	6	5/6	1.190 1.191	1.197	88.88 83.36	97.27 91.52	62.38	69.88

Table S11. Computed [M06/6-311++G(d,p)] B–H terminal bond length (in Å), hydride donating ability (HDA^{MeCN} alias $\Delta G^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol) and enthalpy of hydride detaching reaction ($\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$ in kcal/mol).

Borane	r(B–H)	HDA ^{MeCN}	$\Delta H^\circ_{[\text{H}]^-\text{MeCN}}$
ap-Li ₂ [B ₁₀ H ₁₀]	1.194	102.12	110.69
ap-Li ₂ [B ₅ H ₅]	1.195	96.87	105.74
ap-Li ₂ [B ₁₃ H ₁₅]	1.198	96.55	105.25
ap-Li ₂ [B ₁₇ H ₁₇]	1.187	95.43	103.05
Li ₂ [B ₂ H ₂]	1.187	92.88	100.69
ap-Li ₂ [B ₉ H ₉]	1.201	92.06	100.13
eq-Li ₂ [B ₁₃ H ₁₃]	1.189	91.17	99.75
Li ₂ [B ₁₂ H ₁₂]	1.189	91.13	99.84
ap-Li ₂ [B ₁₀ H ₁₀]	1.194	89.78	98.13
ap-Li ₂ [B ₁₄ H ₁₄]	1.202	89.54	98.01
Li ₂ [B ₆ H ₆]	1.199	89.32	96.64
eq-Li ₂ [B ₇ H ₇]	1.203	89.20	97.12
ap-Li ₂ [B ₁₁ H ₁₁]	1.194	88.20	96.44
ap-Li ₂ [B ₈ H ₈]	1.201	88.07	96.45
eq-Li ₂ [B ₁₄ H ₁₄]	1.189	87.14	95.38
eq-Li ₂ [B ₁₆ H ₁₆]	1.189	87.10	95.19
ap-Li ₂ [B ₁₆ H ₁₆]	1.202	85.33	93.54
eq-Li ₂ [B ₉ H ₉]	1.193	85.10	93.64
eq-Li ₂ [B ₁₅ H ₁₅]	1.190	83.04	91.66
eq-Li ₂ [B ₁₁ H ₁₁]	1.206	78.34	87.15
eq-Li ₂ [B ₅ H ₅]	1.205	75.98	85.00
eq-Li ₂ [B ₈ H ₈]	1.210	75.19	83.50
eq-Li ₂ [B ₁₇ H ₁₇]	1.192	75.11	82.19
ap-Li ₂ [B ₇ H ₇]	1.197	73.55	80.81
Li ₂ [B ₃ H ₃]	1.209	60.85	69.36
ap-Li ₂ [B ₁₃ H ₁₃]	1.192	51.73	60.24
Li ₂ [B ₄ H ₄]	1.205	41.34	49.28

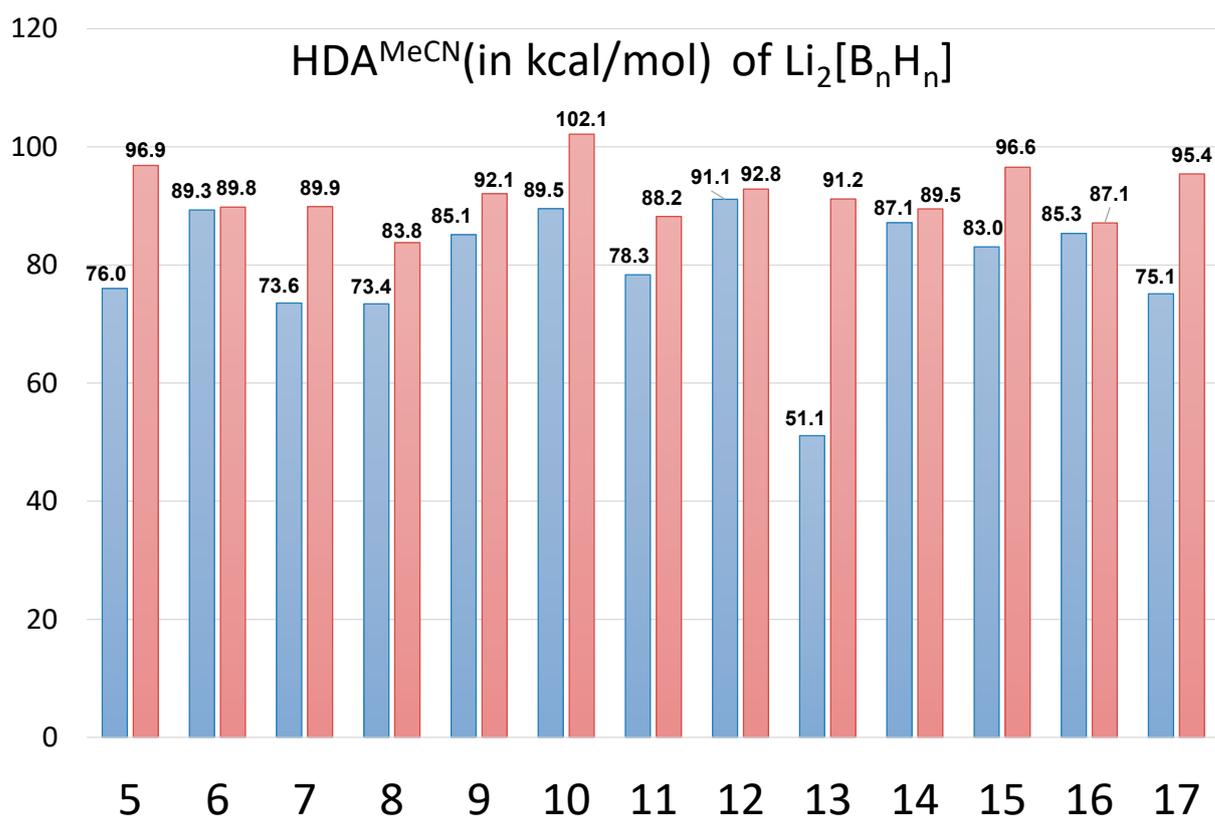
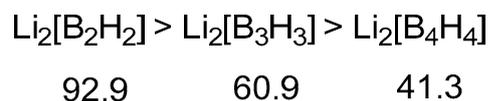
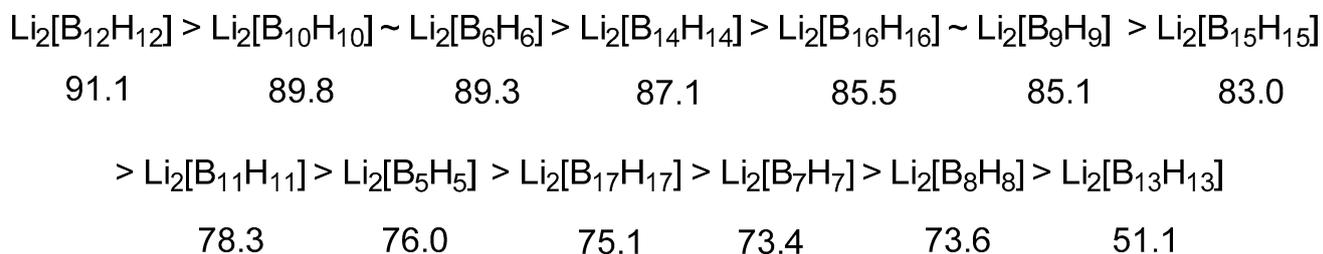


Figure S3. HDA^{MeCN} of polyhedral closo-boranes Li₂[B_nH_n] (n = 5–17). **Blue columns** represent lowest HDA^{MeCN} values, **red columns** – highest.



Scheme S9. General trend of HDA^{MeCN} for Li₂[B_nH_n] (n = 2–4).



Scheme S10. General trend of HDA^{MeCN} for polyhedral closo-boranes Li₂[B_nH_n] (n = 5–17).

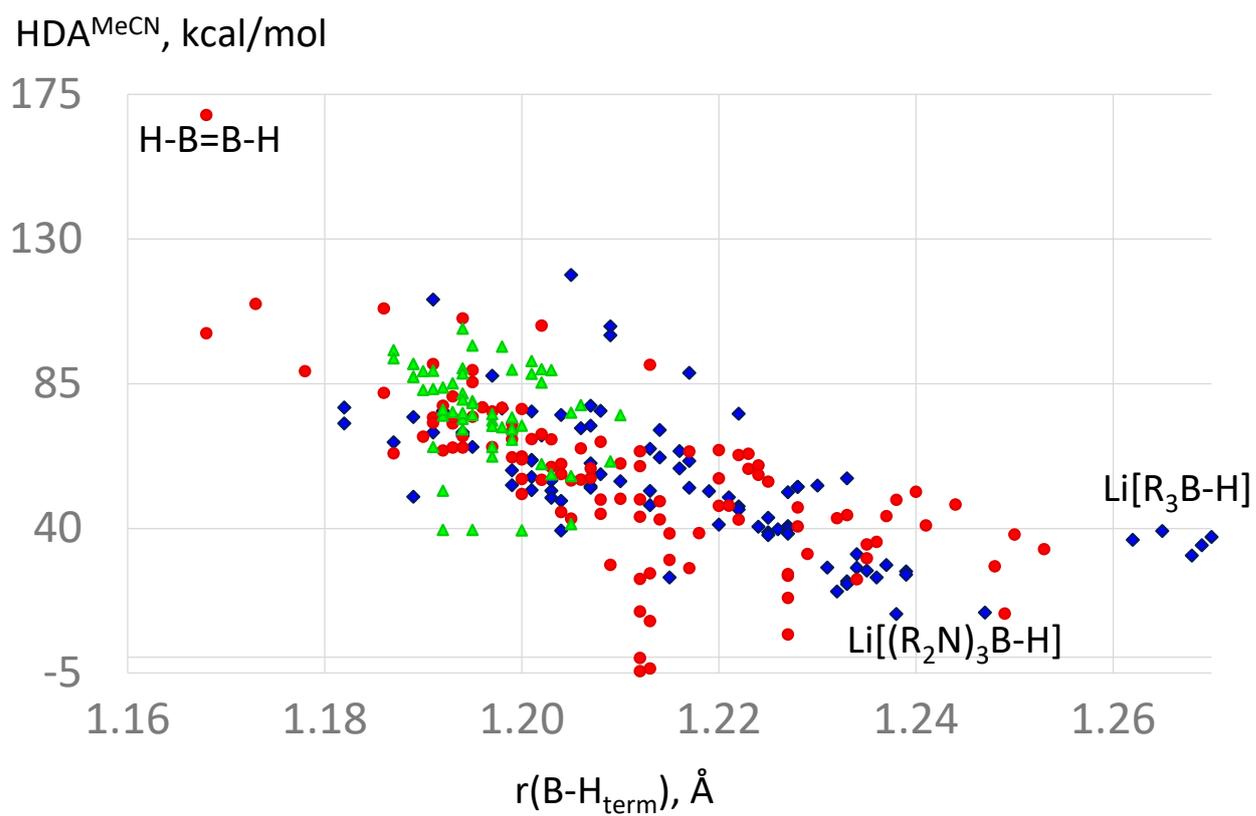


Figure S4. Plot HDA^{MeCN} vs bond length of terminal B-H bond for Li salts polyhedral closo-boranes (green triangles), neutral and anionic borane clusters (red circles) and tetracoordinated boron hydrides (blue squares). HDA^{MeCN} for tetracoordinated boron hydrides are taken from ref.[5]

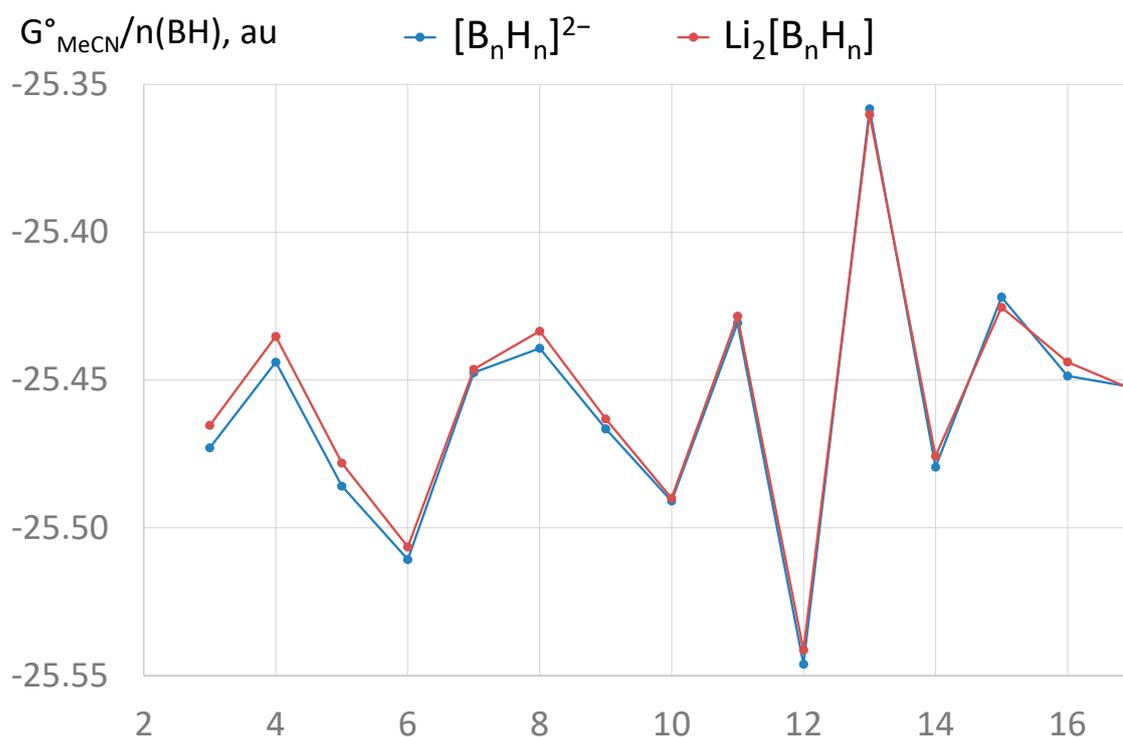


Figure S5. Free Gibbs energy per BH unit calculated for dianions $[B_nH_n]^{2-}$ ($n = 5-17$) of polyhedral closo-boranes and their Li-salts $Li_2[B_nH_n]$ in ($n = 5-17$) MeCN *vs* number boron atoms.

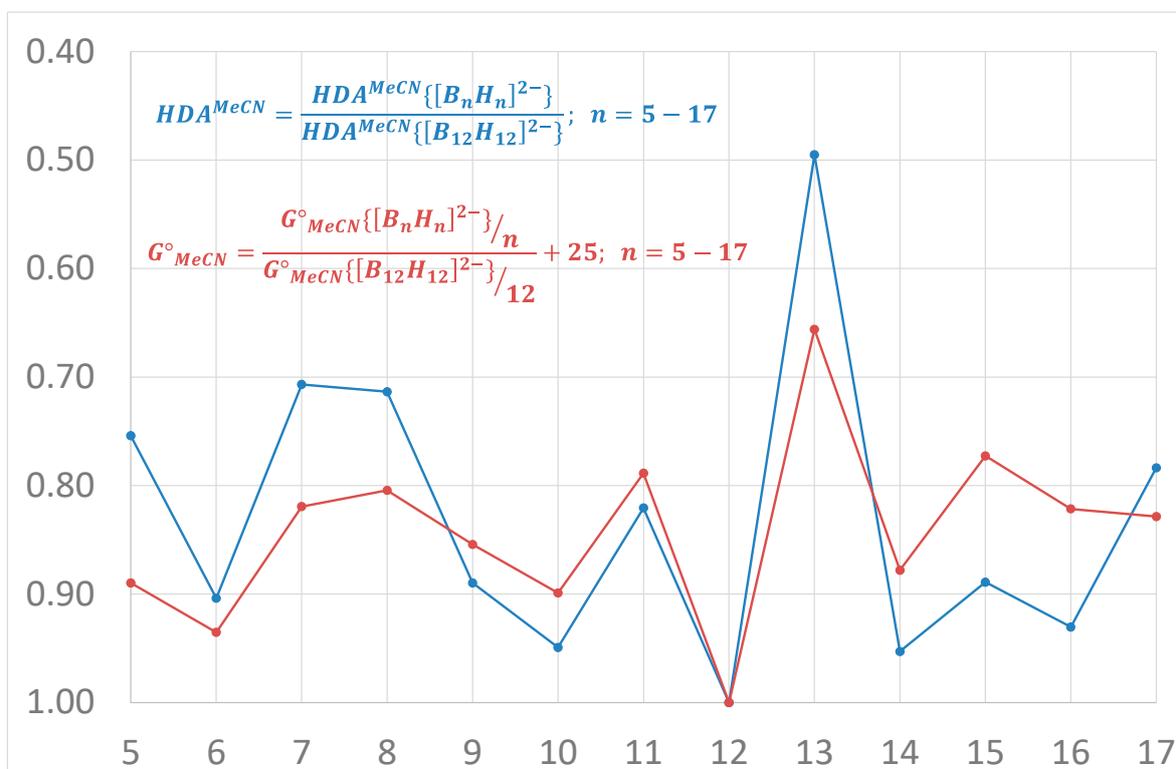


Figure S6. Graph of normalized lowest HDA^{MeCN} of and free Gibbs energy per BH unit for dianions $[B_nH_n]^{2-}$ ($n = 5-17$) of polyhedral closo-boranes *vs* number boron atoms.

Table S12. DFT-optimized geometries (Cartesian coordinates) and electronic energies.

LiBH₄_MeCN E = -34.8014599560 Ha			n-Li[B₅H₁₁]₂_MeCN E = -114.668663978 Ha			n-Li[B₅H₁₀]₂_MeCN E = -141.285709420 Ha			n-Li[B₅H₁₀]₂_MeCN E = -141.285709420 Ha						
5	3.781549000	0.340343000	-0.381731000	5	4.084790000	1.658739000	19.580628000	5	3.957531000	1.742119000	19.470573000	5	6.427795000	2.510349000	21.612823000
1	3.350566000	1.339177000	0.195018000	1	4.483235000	4.822407000	20.495758000	1	4.248691000	2.178410000	20.682038000	1	6.985331000	2.589359000	20.568285000
1	2.993610000	0.071015000	-1.288982000	5	4.532888000	3.537467000	20.562368000	5	4.541384000	3.439856000	20.650461000	1	6.325300000	1.420285000	22.080223000
1	4.852053000	0.651056000	-0.904635000	1	4.630493000	2.231459000	20.614370000	1	4.945229000	1.604050000	18.818656000	5	5.027395000	3.088172000	19.528290000
1	3.914185000	-0.586514000	0.378708000	1	5.009538000	1.256554000	18.941116000	1	2.063547000	4.798502000	21.899153000	5	4.999419000	4.398959000	19.184590000
3	3.557240000	1.936114000	-1.694032000	1	3.238924000	2.201526000	18.953208000	1	5.452754000	3.443264000	21.419271000	1	3.996195000	4.555391000	18.561129000
LiBH₃⁺_MeCN E = -34.0291019103 Ha			{n-Li[B₅H₁₁]₂}⁺_MeCN E = -113.915310391 Ha			{n-Li[B₅H₁₀]₂}⁺_MeCN E = -140.516215454 Ha			{n-Li[B₅H₁₀]₂}⁺_MeCN E = -140.516215454 Ha						
5	3.683581000	0.658581000	-0.359502000	5	4.486441000	3.561478000	20.507604000	5	3.345986000	1.626590000	20.516304000	5	6.574178000	2.361162000	21.648043000
1	3.611936000	0.138848000	0.695153000	1	4.688571000	2.321407000	20.974106000	1	6.220165000	4.326315000	18.370015000	1	7.142942000	2.425511000	20.615681000
1	2.835988000	0.461382000	-1.175646000	5	2.558484000	0.558204000	20.701830000	1	6.367161000	1.312418000	22.162422000	5	5.091983000	4.233359000	19.148370000
1	4.601070000	1.376664000	-0.612984000	1	1.752232000	0.457149000	19.810823000	1	5.240625000	2.869454000	19.321779000	1	6.221304000	4.262704000	18.340978000
3	3.804939000	1.686590000	-2.608552000	1	2.755943000	-0.465435000	21.293120000	1	6.220165000	4.326315000	18.370015000	1	6.220165000	4.326315000	18.370015000
Li[B₂H₇]₂_MeCN E = -61.4282013960 Ha			{n-Li[B₅H₁₀]₂}⁺_MeCN E = -140.522066550 Ha			t-Li[B₅H₁₀]₂_MeCN E = -141.273223117 Ha			t-Li[B₅H₁₀]₂_MeCN E = -141.273223117 Ha						
5	4.071234000	1.657218000	19.959167000	5	3.772427000	1.752151000	19.500853000	5	3.568838000	1.229430000	20.018707000	5	3.568838000	1.229430000	20.018707000
5	4.933726000	3.673993000	20.277279000	1	4.403891000	3.644871000	19.327071000	1	4.682971000	1.783365000	18.735950000	1	4.345922000	3.076720000	20.873542000
1	4.023043000	2.805676000	20.614855000	1	5.439028000	4.039965000	21.028340000	1	2.737626000	2.183458000	19.099016000	1	3.761112000	1.989836000	21.155972000
1	5.173765000	1.194028000	19.760730000	3	0.777120000	2.939467000	21.126105000	1	4.254722000	4.055845000	19.065370000	1	4.611870000	0.680214000	19.760631000
1	3.524956000	1.042687000	20.841323000	1	3.511686000	3.716293000	21.308812000	1	2.063547000	4.798502000	21.899153000	1	2.813365000	0.530200000	20.632478000
1	3.414303000	1.786759000	18.962695000	5	2.548761000	4.288250000	20.694751000	5	1.081069000	3.881654000	22.065177000	1	3.085538000	1.889020000	19.147378000
1	4.348858000	4.643880000	20.674768000	1	2.954746000	5.489685000	20.334477000	1	1.579181000	2.793520000	22.197312000	1	5.024049000	3.209032000	19.917348000
1	5.154234000	3.738573000	19.088418000	1	1.944897000	4.473805000	21.745000000	1	0.760306000	4.369095000	23.112181000	3	6.343884000	1.627501000	19.676597000
1	5.924186000	3.424883000	20.933598000	1	2.015139000	3.762363000	19.841381000	1	0.248341000	3.967461000	21.200796000	1	3.363049000	3.832385000	21.060348000
3	6.553673000	2.408262000	19.376015000	1	4.084029000	0.522696000	20.737603000	1	3.917575000	0.549036000	19.910033000	5	3.535798000	5.081760000	20.427599000
{Li[B₅H₆]₂}⁺_MeCN E = -60.6869426303 Ha			t-Li[B₅H₁₁]₂_MeCN E = -114.656677363 Ha			t-Li[B₅H₁₀]₂_MeCN E = -141.276126434 Ha			{t-Li[B₅H₁₀]₂}⁺_MeCN E = -140.557420018 Ha						
5	4.139542000	1.779815000	20.139773000	5	3.717801000	1.273600000	19.959447000	5	3.244392000	1.124650000	20.080216000	5	4.113447000	4.331566000	17.730951000
5	4.729112000	3.394245000	20.258572000	5	4.296564000	3.178510000	20.868921000	5	4.478454000	2.864779000	20.638820000	5	3.789221000	2.754896000	22.310213000
1	3.599002000	2.923717000	19.771675000	1	3.767921000	2.048442000	21.096326000	1	4.479276000	1.614541000	20.546561000	1	3.633904000	2.973648000	21.164849000
1	5.181834000	2.270615000	20.777645000	1	4.830764000	0.892385000	19.689270000	1	2.554284000	1.034590000	19.252320000	1	3.932524000	3.905473000	18.978210000
1	3.425243000	1.271895000	20.931349000	1	3.074278000	0.458960000	20.561555000	1	2.848311000	1.831031000	19.197482000	1	3.676940000	3.521266000	16.987767000
1	4.485390000	1.148080000	19.186346000	1	3.139980000	1.859988000	19.091816000	3	7.225599000	4.895977000	20.073412000	1	6.869412000	3.163958000	20.612855000
1	4.472638000	4.132450000	21.144001000	1	4.917283000	3.396022000	19.886224000	5	2.771505000	0.056948000	20.430523000				
1	5.442437000	3.772186000	19.377544000	3	6.456242000	2.109615000	19.850131000	1	3.352195000	-0.857806000	20.934485000				
3	5.722593000	2.270636000	17.968345000	1	3.249163000	3.839174000	21.087854000	1	2.262541000	0.800738000	21.233584000				
Li[B₅H₁₀]₂_MeCN E = -88.0414681055 Ha			{t-Li[B₅H₁₁]₂}⁺_MeCN E = -113.915310391 Ha			{t-Li[B₅H₁₀]₂}⁺_MeCN E = -140.557420018 Ha			{t-Li[B₅H₁₀]₂}⁺_MeCN E = -140.557420018 Ha						
5	4.221385000	1.433482000	19.678143000	5	3.901732000	1.692061000	19.878975000	5	4.113447000	4.331566000	17.730951000	5	4.113447000	4.331566000	17.730951000
5	4.701772000	3.378840000	20.539663000	1	3.784461000	1.368136000	21.027617000	1	3.789221000	2.754896000	22.310213000	1	3.789221000	2.754896000	22.310213000
1	4.043760000	2.291606000	20.697672000	1	4.902157000	1.322284000	19.320789000	1	3.633904000	2.973648000	21.164849000	1	3.633904000	2.973648000	21.164849000
1	5.378778000	1.315161000	19.343977000	1	2.914393000	1.732541000	19.220213000	1	3.932524000	3.905473000	18.978210000	1	3.932524000	3.905473000	18.978210000
1	3.875097000	0.500730000	20.352725000	1	6.206420000	1.837911000	21.757607000	1	3.676940000	3.521266000	16.987767000	1	3.676940000	3.521266000	16.987767000
1	3.468488000	1.746976000	18.801989000	1	6.187089000	3.187451000	23.228568000	3	6.869412000	3.163958000	20.612855000	3	6.869412000	3.163958000	20.612855000
1	4.804371000	3.828623000	19.435628000												
1	5.756785000	3.246911000	21.114947000												
3	6.535351000	2.870766000	19.257439000												
1	4.087578000	4.049557000	21.417415000												
5	3.054548000	4.778969000	20.874883000												
1	3.544925000	5.796888000	20.472407000												
1	2.551707000	4.856314000	21.966522000												
1	2.410009000	4.155761000	20.079262000												
{Li[B₅H₆]₂}⁺_MeCN E = -87.2990993667 Ha			{t-Li[B₅H₁₀]₂}⁺_MeCN E = -140.557420018 Ha			{t-Li[B₅H₁₀]₂}⁺_MeCN E = -140.557420018 Ha			{t-Li[B₅H₁₀]₂}⁺_MeCN E = -140.557420018 Ha						
5	4.559742000	2.025562000	19.423394000	5	3.901732000	1.692061000	19.878975000	5	4.113447000	4.331566000	17.730951000	5	4.113447000	4.331566000	17.730951000
5	4.341237000	3.864709000	20.403316000	1	3.784461000	1.368136000	21.027617000	1	3.789221000	2.754896000	22.310213000	1	3.789221000	2.754896000	22.310213000
1	4.725815000	1.645190000	20.556936000	1	4.902157000	1.322284000	19.320789000	1	3.633904000	2.973648000	21.164849000	1	3.633904000	2.973648000	21.164849000
1	5.558781000	2.184532000	18.770401000	1	2.914393000	1.732541000	19.220213000	1	3.932524000	3.905473000	18.978210000	1	3.932524000	3.905473000	18.978210000
1	3.657321000	1.488806000	18.861536000	1	6.206420000	1.837911000	21.757607000	1	3.676940000	3.521266000	16.987767000	1	3.676940000	3.521266000	16.987767000
1	3.947195000	3.239325000	19.376733000	1	6.187089000	3.187451000	23.228568000	3	6.869412000	3.163958000	20.612855000	3	6.869412000	3.163958000	20.612855000
1	5.469381000	4.048371000	20.696422000												
3	6.738948000	2.055004000	20.351646000												
1	3.608816000	3.553875000	21.425882000												

1	2.756526000	3.200502000	22.984523000
5	2.713713000	1.931560000	23.372258000
1	1.713721000	1.468591000	22.947140000
1	3.039748000	1.842613000	24.504697000
1	3.704790000	1.493832000	22.593602000
1	4.651096000	3.426413000	22.951602000
5	5.842461000	2.812625000	22.769211000
1	5.813157000	1.959562000	21.915948000
1	6.050811000	2.407613000	23.869426000
1	6.422863000	3.822075000	22.455913000
1	3.801836000	5.471018000	17.669369000
5	5.232446000	3.838798000	18.940612000
1	5.563339000	2.694046000	19.023108000
1	5.683562000	4.643623000	19.699260000
1	5.439863000	4.248905000	17.721826000

BH₃ MeCN E = -26.5923628927 Ha

5	3.937319000	0.172814000	-0.602166000
1	3.069478000	0.298380000	-1.399609000
1	4.997248000	0.666594000	-0.797230000
1	3.746429000	-0.447554000	0.390721000

BH₂⁺ MeCN E = -25.7531978290 Ha

5	4.001351000	0.379263000	-0.932999000
1	2.900384000	0.169304000	-1.277624000
1	5.102309000	0.589219000	-0.588382000

B₂H₆ MeCN E = -53.2496516866 Ha

5	1.537959000	0.030344000	0.016623000
1	2.170386000	0.314479000	-0.945488000
1	0.681710000	-0.916429000	-0.300370000
1	-0.823693000	-0.245094000	0.895507000
1	-0.726471000	0.328391000	-1.084500000
1	0.665017000	0.985793000	0.250489000
5	-0.191227000	0.039041000	-0.066579000
1	2.073250000	-0.259003000	1.034519000

B₂H₅⁺ MeCN E = -52.4511740928 Ha

5	1.256846000	0.140597000	-0.223046000
1	2.356942000	0.282769000	-0.556667000
1	0.748868000	-0.1010157000	0.208849000
1	-1.258163000	-0.176907000	0.541634000
1	0.205418000	0.356827000	-1.009473000
1	0.692849000	0.812421000	0.778103000
5	-0.157974000	-0.035223000	0.208054000

lin-B₃H₃ MeCN E = -79.8564987956 Ha

5	3.826379000	2.742534000	22.318350000
1	3.662286000	2.947716000	21.171806000
1	2.757473000	3.185902000	22.972622000
5	2.715787000	1.933589000	23.363570000
1	1.729622000	1.455288000	22.918835000
1	3.005596000	1.854029000	24.508266000
1	3.723144000	1.482802000	22.631493000
1	4.648308000	3.444166000	22.971279000
5	5.846296000	2.824468000	22.765989000
1	5.764284000	1.960917000	21.933848000
1	6.050321000	2.441867000	23.882001000
1	6.422980000	3.805314000	22.396574000

lin-B₃H₃⁺ MeCN E = -79.0805617779 Ha

5	4.010320000	2.504940000	22.718649000
1	4.288470000	2.694702000	21.494354000
1	3.055349000	3.259919000	23.084599000
5	5.262131000	2.018563000	23.361412000
1	1.651508000	1.829016000	22.600088000
1	2.480719000	1.899801000	24.529786000
1	3.623751000	1.310738000	22.915214000
1	5.070231000	2.750036000	23.375433000
5	5.492275000	3.013556000	22.089898000
1	6.265010000	2.179688000	21.792887000
1	5.638392000	4.175765000	21.991222000

btf-B₃H₃ MeCN E = -79.8562848596 Ha

5	3.679582000	3.137948000	21.132483000
1	3.889777000	1.999048000	20.906882000
1	2.405488000	3.341902000	20.361622000
5	1.998169000	3.622783000	21.504781000
1	1.190626000	2.804215000	21.808493000
1	1.775776000	4.786569000	21.619108000
1	2.995937000	3.351351000	22.271474000
1	4.861131000	3.467174000	22.009980000
1	4.168986000	3.980619000	20.204481000
5	5.066307000	4.269417000	21.080190000
1	4.870804000	5.393920000	21.418651000
1	6.080685000	3.950238000	20.547440000

btf-B₃H₃⁺ MeCN E = -79.0805381951 Ha

5	3.799397000	3.754632000	21.187222000
1	3.276869000	2.613117000	20.988461000
1	1.546468000	3.470101000	20.261967000
5	2.157389000	3.367920000	21.260425000
1	1.744196000	3.026941000	22.306415000
1	2.843384000	4.549255000	21.452106000
1	4.634702000	3.706616000	22.144831000
1	4.443086000	4.140497000	20.161090000
5	5.441798000	4.142351000	21.113729000
1	5.724412000	5.262422000	21.328944000
1	6.180942000	3.267116000	20.851920000

cyc-B₃H₃ MeCN E = -79.8552502295 Ha

1	-1.062478000	5.525448000	5.008743000
1	0.494385000	6.958134000	5.002293000
5	0.092426000	5.740545000	5.147956000
1	-0.942433000	8.045246000	5.891316000
5	0.062765000	7.456555000	6.131997000
1	-0.457745000	6.798142000	7.127145000
5	0.265437000	5.715945000	7.117669000
1	1.289982000	5.837326000	7.704725000
1	1.030395000	8.072142000	6.438029000
1	0.840003000	5.350900000	4.304174000
1	-0.592632000	5.041375000	7.590524000
1	0.717783000	5.083107000	6.065479000

cyc-B₃H₃⁺ MeCN E = -79.0724553563 Ha

1	-0.977457000	6.054996000	5.168186000
1	0.748350000	7.021658000	5.264942000
5	0.318025000	5.772139000	5.175840000
1	-0.977451000	8.033924000	5.720702000
5	-0.422010000	7.019112000	5.888055000
1	-0.397122000	6.833256000	7.150439000
5	0.286260000	5.662685000	7.169802000
1	1.300016000	5.965003000	7.687896000
1	0.643651000	5.297685000	4.158169000
1	-0.517570000	4.929799000	7.623176000
1	0.702802000	4.962467000	6.084815000

lin-B₃H₃ MP2 MeCN E = -79.2160680965 Ha

5	3.842541000	2.728084000	22.357993000
1	3.711036000	2.977076000	21.212588000
1	2.790682000	3.188916000	23.017628000
5	2.653491000	1.921142000	23.347197000
1	1.669628000	1.515926000	22.822819000
1	2.888525000	1.781062000	24.501184000
1	3.682530000	1.469535000	22.643166000
1	4.673557000	3.331611000	23.092612000
5	5.881604000	2.848018000	22.740417000
1	5.790190000	1.900224000	22.005621000
1	6.226439000	2.585416000	23.859648000
1	6.342252000	3.831914000	22.233759000

lin-B₃H₃⁺ MP2 MeCN E = -78.4882868564 Ha

5	4.011138000	2.504987000	22.720680000
1	4.286883000	2.697604000	21.498137000
1	3.056491000	3.257335000	23.086554000
5	2.511985000	2.013390000	23.367422000
1	1.643942000	1.826185000	22.591121000

1	2.473975000	1.895766000	24.540588000
1	3.625640000	1.312890000	22.918174000
1	5.069912000	2.753015000	23.373311000
5	5.505917000	3.018632000	22.081514000
1	6.271233000	2.170569000	21.788284000
1	5.645041000	4.186353000	21.986848000

btf-B₃H₃ MP2 MeCN E = -79.2055049386 Ha

5	3.678340000	3.149679000	21.135282000
1	3.888203000	2.005681000	20.908538000
1	2.435527000	3.396302000	20.384719000
5	1.984009000	3.615843000	21.530680000
1	1.190942000	2.758123000	21.762490000
1	1.736360000	4.771555000	21.678778000
1	2.973309000	3.332628000	22.288808000
1	4.811752000	3.510449000	22.005079000
1	4.196808000	3.976795000	20.181450000
5	5.080120000	4.278023000	21.054205000
1	4.907703000	5.415983000	21.361316000
1	6.100195000	3.894124000	20.574258000

btf-B₃H₃⁺ MP2 MeCN E = -78.4882573253 Ha

5	3.799510000	3.753891000	21.185370000
1	3.275862000	2.615357000	20.986732000
1	1.535643000	3.470476000	20.255374000
5	2.141542000	3.364572000	21.261720000
1	1.739758000	3.024455000	22.317323000
1	2.845210000	4.547330000	21.449128000
1	4.632959000	3.705172000	22.141539000
1	4.444206000	4.138569000	20.162337000
5	5.457755000	4.146339000	21.114056000
1	5.728200000	5.273431000	21.332425000
1	6.191998000	3.261377000	20.851105000

cyc-B₃H₃ MP2 MeCN E = -79.2060007087 Ha

1	-1.060786000	5.510346000	4.968243000
1	0.464322000	6.957315000	5.010597000
5	0.093265000	5.728516000	5.124106000
1	-0.955198000	8.057768000	5.900741000
5	0.058625000	7.479162000	6.133627000
1	-0.426779000	6.801038000	7.127486000
5	0.268485000	5.705272000	7.138439000
1	1.306730000	5.824381000	7.704695000
1	1.036660000	8.088304000	6.429159000
1	0.877957000	5.354561000	4.304219000
1	-0.598650000	5.043169000	7.616981000
1	0.672231000	5.075033000	6.071756000

cyc-B₃H₃⁺ MP2 MeCN E = -78.4715043739 Ha

1	-0.973753000	6.055804000	5.170755000
1	0.750035000	7.014697000	5.278819000
5	0.319526000	5.769707000	5.159004000
1	-0.982698000	8.053118000	5.705586000
5	-0.429914000	7.032479000	5.879995000
1	-0.398360000	6.814046000	7.136299000
5	0.292867000	6.562052000	7.194757000
1	1.314342000	5.968227000	7.697169000
1	0.648001000	5.300558000	4.134260000
1	-0.515601000	4.917453000	7.646467000
1	0.683049000	4.9745851000	6.088911000

lin-B₃H₃⁺ MeCN E = -106.468663139 Ha

5	4.208856000	2.733282000	22.093432000
1	3.759273000	3.344219000	21.196951000
1	2.400965000	3.119466000	23.261193000
5	2.701049000	1.961874000	23.261797000
1	1.884549000	1.210076000	22.850345000
1	3.651931000	1.622137000	22.39529200

5	-0.01559000	6.63792800	4.18851000
1	-1.19245800	6.63792200	4.18986600
1	0.52454700	7.06232600	3.21259800

cyc-B₅H₁₁⁺ MeCN E = -105.684419501 Ha

1	-0.72109600	5.49672800	4.85811000
1	1.18915900	5.52829500	4.31707600
5	0.39552600	4.86533200	5.14927400
1	-1.17560000	7.32642400	5.96115600
5	-0.00449900	7.42973900	6.08378200
1	0.69909900	6.79834000	6.97745900
5	0.28703200	5.56702800	7.02926600
1	0.94371500	5.27936500	7.97447900
1	0.43992700	8.49997900	6.33808500
1	0.26515000	3.75453000	4.80453700
1	-0.84718900	5.23682700	7.01535300
1	1.11213500	4.93876600	6.21807200
1	0.72738300	7.34239200	4.99348400
5	0.15498800	6.35791200	4.39068600
1	-0.20379600	6.67270700	3.32213900

lin-B₅H₁₅ MeCN E = -133.082511176 Ha

5	4.12782500	2.78148200	22.01607600
1	3.61670100	3.43349000	21.18476300
1	2.42832800	3.14717000	23.36348800
5	2.71716400	1.99333800	23.27077400
1	1.86119300	1.24275700	22.94863700
1	3.56504200	1.66538200	22.31529000
1	4.66185700	3.48281700	22.95923900
5	5.75832700	2.82124500	22.56530500
1	5.19961200	2.20113000	21.53238900
1	6.06013100	2.03556300	23.39537100
1	6.50014800	3.63078500	22.13162400
1	3.37146400	1.83757000	24.34335200
5	3.50224600	0.50560900	24.66412300
1	3.88583500	-0.14628600	23.75166500
1	2.51377600	0.19895900	25.24471800
1	4.36606500	1.01531300	25.44913200
5	5.24061200	0.05664500	25.89952300
1	6.17306500	0.13881600	25.14977000
1	5.37046000	0.61147600	26.95825200
1	4.70915900	-0.10167200	25.96173900

lin-B₅H₁₄⁺ MeCN E = -132.332277713 Ha

5	4.65528200	2.22840000	22.57811000
1	4.32069200	1.25338300	22.01845800
1	2.49327800	2.52051700	23.33206800
5	3.31027900	2.18053500	24.11778300
1	4.57680100	2.37660200	23.86752800
1	4.30452600	3.31564000	21.98231900
5	5.63327600	3.52257800	22.01898500
1	5.94769400	2.33837400	22.57851600
1	5.87463800	4.39845400	22.77028700
1	6.01908500	3.48346600	20.90491300
1	3.32654400	2.69201300	25.18710800
5	3.44433000	0.42355600	25.17797100
1	3.11427700	0.90093200	24.01147100
1	2.56840700	0.35657600	25.95365400
1	4.56507800	0.76177000	25.70933700
5	4.96040000	-0.37755600	25.10498400
1	5.63774300	-0.11601900	24.17326500
1	5.27760700	-1.11481500	25.96859000
1	3.73787900	-0.75062000	24.70224700

iso-B₅H₁₅ MeCN E = -133.074163066 Ha

5	4.23872300	2.21923300	22.37006800
1	2.81010800	3.08325600	24.23927700
5	2.89789100	1.89313400	24.15853000
1	3.38941200	1.34303600	25.10362900
1	4.03533200	1.52400300	23.38054600
1	4.55760500	3.41080300	22.85862700

5	5.83039200	3.49301700	22.70090100
1	5.09280000	1.64370900	21.78288600
1	6.24741400	3.82909500	21.65745600
1	2.00663700	1.32178400	23.60332900
1	3.26789700	2.75822900	21.81449200
5	2.89078500	2.00482500	20.67492000
1	1.81698400	2.53436900	20.75667700
1	3.60904200	2.37512400	19.79470900
1	2.90938900	0.83932600	20.94662600
1	6.53754300	2.57819800	23.27263200
5	6.55800700	3.49177100	24.25765700
1	5.95514400	4.46276800	23.57012900
1	5.87044900	3.13110300	25.14785700
1	7.68665600	3.81154500	24.38654600

iso-B₅H₁₄⁺ MeCN E = -132.305697001 Ha

5	3.98433300	2.12248300	23.07391000
5	2.50641400	2.00982800	23.92782100
1	2.41514900	2.56523900	24.96096200
1	3.62657500	1.23243600	23.42772600
1	4.85791300	2.67234500	23.86728100
5	5.53207000	3.43936600	23.04417300
1	4.33017600	1.62277600	22.05860100
1	4.99580100	4.09294200	22.23107200
1	1.65491400	1.37312400	23.42015000
1	2.95967300	2.88359600	22.98726300
5	3.38260500	1.90417500	20.25339000
1	2.43994500	1.58909000	20.57657500
1	3.33647200	3.08938500	20.31456200
1	4.34531800	1.37174300	19.80749600
1	6.51376400	2.75069600	22.59470700
5	7.14326700	3.38743800	23.61617400
1	6.06100100	4.13755700	23.98136700
1	7.40065000	2.61667800	24.46749400
1	7.91206200	4.13435500	23.12749300

pinc-B₅H₁₅ MeCN E = -133.068649074 Ha

5	4.23758100	2.52945800	22.06873200
1	2.40463900	3.15156100	23.15482000
5	2.64294000	1.98738600	23.28080700
1	1.81604400	1.22570600	22.91202000
1	3.57252000	1.51521600	22.41192400
1	4.69679800	3.30646600	23.00358700
5	5.82550900	2.64542600	22.71123000
1	5.33121000	1.91604800	21.71608500
1	6.07365500	1.92697400	23.62024300
1	6.57989600	3.42365100	22.25326600
1	3.21488000	1.95250700	24.39456100
5	3.28843300	0.65972000	24.90407900
1	3.74115200	-0.09936800	24.09563300
1	4.08126100	1.06348000	25.71356900
1	2.20212700	0.39861400	25.33304600
1	3.85524300	3.36477700	21.24587300
5	3.39380400	2.65637100	20.07744300
1	3.77217000	1.52141700	20.11594400
1	2.22620000	2.83085700	20.25099800
1	3.98640500	3.38740600	19.34466200

pinc-B₅H₁₄⁺ MeCN E = -132.308414181 Ha

5	4.32637800	3.14377100	23.23185200
1	4.29025200	3.69148100	24.26670800
5	2.79741600	1.88817600	23.64391100
1	2.04071500	2.77533600	23.51173000
1	3.98648900	1.89132700	23.10346400
1	5.54021300	2.92424500	22.86217000
5	5.06183600	3.57498000	21.75255900
1	5.00290900	2.82759100	20.82638600
1	5.63849600	4.59699400	21.67057600
1	2.95041700	1.51332100	24.85874800
5	2.64642800	0.31396700	24.29231300
1	2.40577500	0.82016600	23.04863300

1	3.60172400	-0.37392200	24.26979800
1	1.59711800	-0.00359900	24.72356500
1	3.83983900	3.83434300	22.25723600
5	3.81184100	1.53441200	20.18993000
1	4.23685600	0.69797500	20.92052100
1	2.80389000	2.09806400	20.47318000
1	4.29526700	1.68852500	19.11684400

cyc-B₅H₁₅ MeCN E = -133.069556321 Ha

1	-0.91404400	4.50081100	5.13369200
1	1.06888100	4.52324300	4.24013100
5	0.23915800	4.28872200	5.22896100
1	-0.98244900	8.13466900	6.10666900
5	0.02929800	7.51367500	6.15663000
1	-0.50725400	6.41311000	6.60528900
5	0.36956200	5.51153200	6.95672300
1	1.32047100	5.82629100	7.59086800
1	0.93441500	8.00754400	6.74238800
1	0.60217500	3.18358700	5.47449400
1	-0.40972000	4.78197700	4.78328000
1	1.02018400	5.08627300	5.92956700
5	0.54050000	5.20860300	3.27177400
1	-0.49727300	4.89107400	2.21362000
1	1.50804000	5.07381700	2.57962000
1	0.67752900	7.30935600	5.05959100
5	-0.17793900	7.11145600	4.07936000
1	-1.22475700	6.61154800	4.27211300
1	0.81164300	6.45323200	3.51712000
1	-0.12469900	8.10089100	3.42265600

cyc-B₅H₁₄⁺ MeCN E = -132.300360632 Ha

1	-0.84926800	4.75823100	4.79199500
1	1.25082500	4.59096600	4.16794800
5	0.52379400	4.38853000	5.27278300
1	-0.84205300	8.23900100	6.27740600
5	0.10405000	7.53362400	6.17748200
1	-0.50001300	6.43527800	6.54419100
5	0.31733300	5.49899700	6.92167000
1	1.07779600	5.66475000	7.80490800
1	1.12630700	7.86331900	6.67286100
1	0.57050700	3.24539600	5.51117700
1	-0.53741900	4.67775800	7.06501500
1	1.20771100	5.23961200	5.98229100
5	0.10822000	5.10729300	7.75966000
1	-0.28986800	4.55660200	2.82145500
1	0.63343300	7.38965800	4.99193500
5	-0.30350600	7.17444300	4.12637300
1	-1.39859300	6.79699700	4.35308000
1	0.50404300	6.28570600	3.51101000
1	-0.12761800	8.01140400	3.30917000

Li₂BH₃ MeCN E = -41.6940037919 Ha

5	3.19494300	6.30719400	4.72167200
1	2.28760200	6.88967800	5.30147100
1	3.18417100	5.10536100	5.01398000
1	4.28954700	6.75330100	5.08484500
3	1.80963000	7.18953500	3.22296900
3	4.71110400	5.33321100	3.75166500

{Li₂BH₂}⁺ MeCN E = -40.9539413983 Ha

5	2.99911000	6.06216200	4.77378700
1	2.05488700	6.68154900	5.23107000
1	3.43679800	5.37268400	5.66216600
3	2.19182900	7.33385200	3.13524200
3	4.50482600	5.37473300	3.20949200

Li₂[B₂H₄] MeCN E = -68.4069532578 Ha

5	3.23984800	6.30047400	2.79205900
1	3.26849300	7.46704200	2.37197200
1	4.17452000	5.70556000	2.25504200
1	2.19405100	5.80902400	2.34029400
5	3.23062400	6.27151200	4.57929100
1	2.29624000	6.86650800	5.11654100

1	3.20177300	5.10484600	4.99923800
1	4.27665900	6.76260100	5.03091300
3	1.57987400	7.36973800	3.41559200
3	4.89182600	5.20307600	3.95502800

{Li₂B₂H₅}⁺ MeCN E = -67.6748063751 Ha

5	3.30831700</
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1	-0.584311000	4.923590000	7.287935000
1	1.300668000	4.796357000	6.487868000
3	1.203233000	7.944873000	4.383329000
3	0.360033000	3.227637000	7.327369000
7,2-Li₂[BaH₁₂]₂ MeCN E = -121.668798779 Ha			
5	0.364945000	-0.251558000	1.405122000
1	1.567085000	-0.243885000	1.565015000
1	-0.187140000	-0.405923000	2.479361000
1	0.153381000	1.074820000	1.427558000
3	-1.892414000	0.048669000	1.283450000
5	-0.289848000	-1.290076000	0.161619000
1	-1.509131000	-1.357335000	0.104526000
1	0.087672000	-1.153103000	-0.986958000
3	1.750786000	-0.507512000	-0.371843000
5	-0.093188000	1.604899000	0.264351000
1	0.724986000	1.346159000	-0.586270000
1	0.020754000	2.735478000	0.672718000
1	-1.229600000	1.361403000	-0.088017000
1	-0.210473000	-2.572871000	0.433901000
5	1.003383000	-3.020779000	0.689784000
1	1.916253000	-2.488711000	0.099356000
1	1.120542000	-2.987396000	1.887750000
1	0.794157000	-4.125339000	0.246333000

{1,2-Li₂[BaH₁₁]}* MeCN E = -120.946310331 Ha			
5	0.781056000	-0.527440000	0.933558000
1	1.892945000	-0.159169000	0.676012000
1	0.928717000	-0.983844000	2.077491000
1	0.001317000	0.376457000	1.387063000
3	-1.563005000	0.476529000	-1.210678000
5	-0.004809000	-1.609154000	-0.238175000
1	-1.130247000	-1.267542000	-0.502501000
1	0.692780000	-1.822605000	-1.201559000
3	1.973071000	-0.407709000	-1.204175000
5	-0.208912000	1.358304000	0.498569000
1	0.232584000	1.236422000	-0.621644000
1	0.272817000	2.276063000	1.090434000
1	-1.418337000	1.310655000	0.544464000
1	-0.175651000	-2.772396000	0.200547000
5	0.315007000	-2.193995000	1.417039000
1	-0.636209000	-2.305275000	2.124475000
1	1.243718000	-2.917514000	1.606373000

7,1-Li₂[BaH₁₂]₂ MeCN E = -121.661148790 Ha			
5	3.984956000	2.248559000	22.213019000
1	3.725041000	3.158030000	21.428695000
1	2.317838000	3.043583000	23.955186000
5	2.726147000	2.041116000	23.385551000
1	4.215820000	1.260381000	21.531948000
1	5.028715000	2.588296000	22.795181000
1	2.941766000	1.474205000	24.570532000
5	3.629929000	0.364765000	24.579076000
1	3.523496000	-0.320624000	23.590270000
1	4.767306000	0.717513000	24.815304000
1	3.094398000	-0.126032000	25.537489000
3	3.572269000	4.212462000	22.996898000
3	5.260901000	0.559661000	22.938080000
1	1.654973000	1.336862000	23.255009000
5	1.085980000	1.431955000	22.057038000
1	1.105922000	2.552622000	21.624046000
1	0.004069000	1.108555000	22.488146000
1	1.607301000	0.600135000	21.361534000

{1,1-Li₂[BaH₁₁]}* MeCN E = -120.946307002 Ha			
5	3.224374000	1.982452000	22.004635000
1	3.798543000	3.034627000	21.850561000
1	2.418050000	2.855036000	24.272961000
5	2.370436000	1.890675000	23.561096000
1	3.904553000	1.009960000	21.795182000
1	2.524500000	0.770789000	24.155572000
5	3.733929000	0.660273000	24.725356000

1	4.020174000	-0.395796000	24.205877000
1	4.551497000	1.528758000	24.523574000
1	3.413455000	0.579566000	25.872306000
3	3.916370000	3.797592000	23.596395000
3	5.297096000	0.454115000	22.984320000
1	1.146450000	1.695844000	23.492803000
5	1.452128000	1.763370000	22.021517000
1	0.752332000	2.701917000	21.795168000
1	1.055735000	0.682487000	21.717552000
1	2.451385000	1.979998000	21.016178000

lin-Li₂[BaH₁₂]₂ MeCN E = -121.660350782 Ha			
5	4.431678000	2.648978000	22.087925000
1	3.709032000	3.602105000	22.195699000
1	1.760910000	2.084687000	22.450116000
5	2.586031000	1.377194000	22.949757000
1	2.348999000	0.206281000	22.898726000
1	3.752909000	1.463100000	22.496966000
1	5.785515000	3.178814000	24.122381000
5	5.885111000	2.604300000	23.046418000
1	4.484685000	2.302897000	20.912548000
1	6.288675000	1.442055000	23.239825000
1	6.800721000	3.161275000	22.437545000
1	2.594683000	1.956693000	24.108663000
5	3.091322000	1.189936000	25.062834000
1	3.927646000	0.386454000	24.725916000
1	2.152702000	0.686109000	25.608939000
1	3.558233000	2.129703000	25.677405000
3	5.418073000	1.592126000	25.026731000
3	6.342469000	1.762019000	21.144484000

{lin-Li₂[BaH₁₁]}* MeCN E = -120.924331997 Ha			
5	4.461404000	2.050639000	22.134349000
1	3.338384000	2.792324000	22.345449000
5	2.962539000	1.709421000	22.932507000
1	1.932251000	1.316916000	22.515356000
1	3.914957000	0.916435000	22.632657000
1	5.495228000	3.174270000	24.028143000
5	5.830448000	2.509219000	23.057803000
1	4.414966000	1.851135000	20.947953000
1	6.379224000	1.469662000	23.428644000
1	6.686494000	3.169000000	22.480039000
1	2.948034000	2.147828000	24.112328000
5	3.168143000	2.121204000	25.111274000
1	3.939411000	0.364394000	24.752404000
1	2.073399000	0.844312000	25.395224000
1	3.637966000	2.058804000	25.830873000
3	5.568346000	1.665220000	25.221136000
3	6.407292000	2.437457000	20.816624000

pinc-Li₂[BaH₁₅]₂ MeCN E = -148.286835846 Ha			
5	3.714258000	2.353175000	22.260355000
1	3.139744000	3.201492000	21.601810000
1	2.879787000	3.023073000	24.560447000
5	2.924058000	1.203865000	23.776455000
1	3.859420000	1.370985000	21.560577000
1	4.929427000	2.849519000	22.064820000
5	5.594851000	3.113667000	23.153567000
1	5.819962000	2.134924000	23.828891000
1	5.096054000	4.016104000	23.785662000
1	6.565537000	3.474088000	22.533633000
1	3.345649000	1.323394000	24.724902000
5	3.436655000	0.020441000	24.482680000
1	3.134071000	-0.331957000	23.373688000
1	4.168641000	-0.105814000	24.725345000
1	2.720217000	-0.395696000	25.346362000
3	3.100349000	4.376957000	23.225356000
3	5.027635000	0.468994000	22.872366000
1	1.803891000	1.583893000	23.437959000
5	0.732970000	2.358708000	23.711264000
1	0.033298000	1.659739000	23.020807000

1	0.493119000	2.308404000	24.885562000
1	0.879308000	3.469361000	23.259144000
{pinc-Li₂[BaH₁₅]}* MeCN E = -147.561523802 Ha			
5	3.700948000	1.615513000	22.475711000
1	3.167826000	2.169911000	21.574878000
1	3.208664000	2.154133000	24.835827000
5	2.700796000	1.564655000	23.931730000
1	4.040019000	1.507049000	22.015183000
1	4.942201000	1.894982000	22.708809000
5	5.128182000	3.160714000	23.026139000
1	5.486957000	3.045679000	24.178828000
1	4.238787000	3.947450000	22.870719000
1	6.014847000	3.382468000	22.232693000
1	5.202413000	0.444669000	24.437027000
5	3.328362000	0.049901000	23.233698000
1	2.531787000	-0.642064000	22.683388000
1	4.223324000	-0.465485000	23.826073000
3	3.080214000	4.104583000	24.521615000
3	7.398782000	3.180919000	23.618477000
1	1.476995000	1.741569000	23.818652000
5	1.088456000	3.035671000	23.767138000
1	0.035790000	2.815852000	23.241989000
1	1.031475000	3.297199000	24.938991000
1	1.783869000	3.767445000	23.107725000

7,2-Li₂[BaH₁₅]₂ MeCN E = -148.284984930 Ha			
5	4.491812000	2.417905000	21.972703000
1	4.189543000	3.249787000	21.157265000
1	2.490265000	3.109729000	23.671809000
5	2.629902000	1.991676000	23.270482000
1	1.620810000	1.412386000	22.992234000
1	3.237230000	1.894520000	22.167438000
1	4.933785000	3.926572000	23.874794000
5	5.463496000	3.021994000	23.266163000
1	4.855551000	1.390307000	21.417272000
1	5.997806000	2.241061000	24.049514000
1	3.278139000	1.541990000	24.289684000
5	3.442931000	0.218148000	24.268215000
1	3.572610000	-0.259612000	23.169833000
1	2.550576000	-0.252109000	24.908216000
1	4.491664000	0.285099000	24.876634000
3	6.240906000	3.874028000	25.239884000
3	5.477875000	0.581781000	23.093471000
1	6.446490000	3.407431000	22.485727000
5	7.200460000	4.417426000	22.898699000
1	6.626153000	5.436901000	22.629583000
1	8.107820000	4.143336000	22.152795000
1	7.588360000	4.348439000	24.045987000

{1,2-Li₂[BaH₁₄]}* MeCN E = -147.545868019 Ha			
5	4.496744000	2.511483000	22.018548000
1	4.143532000	3.294159000	21.174728000
1	3.053740000	3.195297000	24.194234000
5	2.944134000	2.141432000	23.616211000
1	1.810149000	1.781761000	23.537703000
1	3.226867000	2.193473000	22.381244000
1	5.611923000	4.464832000	23.112867000
5	5.646357000	3.132041000	23.104352000
1	4.760572000	1.454437000	21.481312000
1	5.783843000	2.791741000	24.254520000
1	3.745544000	1.421433000	24.292141000
5	3.586264000	0.093293000	24.147141000
1	3.227994000	-0.231692000	23.044927000
1	2.873065000	-0.254586000	25.035680000
1	4.768483000	-0.094861000	24.356187000
3	4.433882000		

1	5.237688000	-0.840362000	25.801345000
3	5.784765000	2.538043000	25.077759000
3	6.346673000	1.013933000	22.285084000
{lin-Li₂[B₅H₁₄]}* MeCN E = -147.559743641 Ha			
5	4.307122000	2.263314000	21.676915000
1	3.698103000	2.805259000	20.812468000
5	3.369392000	2.263045000	23.228572000
1	2.664809000	3.051104000	23.771014000
1	2.741826000	1.623616000	22.424289000
1	4.795418000	4.333069000	23.144598000
5	4.958381000	3.164722000	22.994809000
1	4.734700000	1.176924000	21.395831000
1	5.807231000	2.650159000	23.687795000
1	5.425357000	3.039263000	21.803998000
1	3.800932000	1.559619000	24.250448000
5	3.516603000	0.302418000	24.232449000
1	4.092814000	-0.337841000	23.405569000
1	2.357505000	0.067566000	24.354064000
1	3.840600000	0.064312000	25.456837000
5	5.122986000	0.214928000	25.794080000
1	5.923034000	0.509088000	24.937939000
1	4.967950000	1.085834000	26.621810000
1	5.316686000	-0.869916000	26.253469000
3	6.063489000	2.500090000	25.838478000
3	5.837648000	0.440647000	22.838767000
LiBH₂ MeCN E = -33.499097138 Ha			
5	1.877261000	-0.366328000	-0.398690000
1	1.860027000	0.578727000	-1.169552000
1	2.305226000	0.081071000	0.652499000
3	1.250201000	-2.508100000	-0.825288000
{LiBH₃}* MeCN E = -32.7368703398 Ha			
5	1.735538000	-0.416774000	-0.823000000
1	1.980458000	0.752929000	-0.908301000
3	1.271493000	-2.631856000	-0.662229000
Li[B₂H₃]* MeCN E = -60.2207886654 Ha			
5	1.469485000	-0.040700000	0.210726000
1	2.159246000	0.439963000	-0.669670000
1	0.685268000	-0.989553000	-0.377242000
1	-0.852204000	-0.546270000	0.946064000
1	-0.733117000	0.459019000	-0.810528000
5	-0.138865000	-0.003107200	0.132181000
1	2.092872000	-0.567237000	1.088802000
3	0.725349000	1.764681000	-0.925635000
{Li[B₂H₄]}* MeCN E = -59.4509061030 Ha			
5	1.545279000	-0.065217000	-0.258367000
1	2.585806000	-0.078801000	-0.784815000
1	0.673986000	-1.048910000	-0.464678000
1	-0.719137000	-0.346116000	1.038534000
5	0.269462000	-0.166857000	0.446857000
1	1.448435000	-0.329693000	1.043327000
3	0.337319000	2.065406000	-0.615632000
Li[B₃H₃]* MeCN E = -86.8815377270 Ha			
1	-0.756758000	5.181923000	4.888354000
1	-0.045402000	6.976828000	4.703045000
5	0.156859000	5.866186000	5.244923000
1	-0.982345000	8.026554000	6.140750000
5	0.030604000	7.395080000	6.135536000
1	-0.002196000	7.022421000	7.582288000
5	0.183947000	5.895145000	7.069993000
1	1.274911000	5.569040000	7.483541000
1	1.043601000	8.052740000	6.110020000
1	1.235412000	5.514946000	4.810185000
1	-0.718380000	5.223309000	7.475506000
3	2.292560000	6.364174000	6.119409000
{Li[B₃H₄]}* MeCN E = -86.1069241752 Ha			
1	-0.372615000	4.807165000	5.080611000
5	0.377862000	5.559215000	5.609560000

1	-0.972529000	7.998999000	6.273380000
5	0.037003000	7.374872000	6.288318000
1	0.286552000	7.037209000	7.596900000
5	-0.237278000	5.958199000	7.088097000
1	0.657794000	5.504287000	6.852989000
1	1.001360000	7.968089000	5.926811000
1	1.433897000	5.683972000	5.077231000
1	-1.195939000	5.573497000	7.644870000
3	2.742107000	7.095287000	5.621736000
Li[B₃H₅]* MeCN E = -86.8781378642 Ha			
1	-0.763003000	5.255547000	4.924429000
1	-0.781492000	7.190534000	4.799506000
5	-0.080207000	6.235839000	5.089966000
5	0.279998000	7.148636000	6.664077000
1	-0.650561000	7.700418000	7.171415000
5	0.275249000	5.445575000	6.721496000
1	0.804617000	6.352941000	7.562550000
1	1.1212543000	7.865839000	6.385840000
1	0.913466000	6.182677000	4.381509000
1	-0.654249000	4.967431000	7.300925000
1	1.201739000	4.728659000	6.487230000
3	1.062454000	8.035711000	4.416281000
{Li[B₃H₆]}* MeCN E = -86.1090897476 Ha			
1	-0.380325000	7.583303000	4.878814000
5	0.440483000	6.923306000	5.452762000
5	0.143389000	6.985240000	7.070758000
1	-0.621002000	7.615781000	7.699607000
5	0.146896000	5.396137000	6.625271000
1	0.746392000	6.031945000	7.703637000
1	0.996180000	7.172410200	6.392669000
1	1.366413000	6.501211000	4.834024000
1	-0.875492000	4.946195000	7.034007000
1	0.961739000	4.663165000	6.185331000
3	0.658886000	7.483875000	3.103914000
{lin-Li[B₄H₁₁]}* MeCN E = -113.497521659 Ha			
1	-1.089837000	5.055681000	5.045196000
1	0.072292000	6.564962000	4.671829000
5	-0.025584000	5.504864000	5.349740000
1	-0.838338000	7.849525000	5.948510000
5	0.098157000	7.117790000	6.024804000
1	0.176442000	6.989046000	7.478288000
5	0.036104000	5.777706000	7.152162000
1	1.009908000	5.255309000	7.638886000
1	0.920893000	4.857433000	4.971597000
1	-1.001973000	5.455460000	7.647978000
3	2.295546000	5.171269000	6.244893000
1	1.057044000	7.930908000	5.865129000
5	2.380066000	7.540542000	5.876962000
1	2.545961000	6.795676000	4.949669000
1	2.762698000	6.858015000	5.697884000
1	2.616859000	7.097057000	6.967807000
{lin-Li[B₄H₁₂]}* MeCN E = -112.760825298 Ha			
1	-1.192226000	5.151819000	5.708572000
1	-0.048954000	6.446118000	4.601044000
5	-0.070470000	5.531323000	5.683255000
1	-0.638390000	8.174629000	5.431523000
5	0.180995000	7.326250000	5.466781000
1	-0.228265000	7.122961000	7.880184000
5	0.443167000	6.654438000	7.030211000
1	0.727460000	4.767346000	5.217652000
1	0.355897000	5.401257000	7.032358000
3	2.774577000	4.778666000	5.083046000
1	1.248557000	7.710862000	4.927489000
5	1.861497000	7.422122000	6.173488000
1	2.731016000	6.729108000	5.725384000
1	2.205490000	8.482702000	6.573268000
1	1.655972000	6.666334000	7.358193000
cyc-Li[B₄H₁₁]* MeCN E = -113.468317653 Ha			

1	-1.700353000	4.894422000	5.082444000
5	-0.511833000	5.056504000	4.972324000
1	-1.405139000	7.139422000	6.361847000
5	-0.251256000	7.393758000	6.247626000
1	0.512494000	6.692491000	7.033959000
5	0.653062000	5.459605000	6.663802000
1	1.706846000	5.389427000	6.095506000
1	0.091971000	8.436148000	6.740349000
1	0.002871000	4.049427000	4.510427000
1	0.699020000	4.992660000	7.769930000
1	-0.380055000	4.821549000	6.297388000
1	0.290299000	7.611702000	5.119025000
5	-0.067921000	6.596748000	4.313760000
1	-0.898563000	7.124327000	3.620478000
1	1.033434000	6.992375000	3.781775000
3	1.600483000	4.947772000	4.139005000
{cyc-Li[B₄H₁₁]}* MeCN E = -112.760817295 Ha			
1	-0.995885000	5.552512000	4.642505000
5	-0.918958000	5.870909000	5.856222000
1	-1.992531000	5.972307000	6.335542000
5	0.106550000	7.230769000	6.110678000
1	1.220101000	6.907884000	6.592908000
5	0.675822000	5.602270000	6.705233000
1	1.565354000	5.051004000	6.119647000
1	-0.386906000	8.100982000	6.736818000
1	0.630821000	5.416271000	7.874238000
1	-0.376856000	4.791157000	6.200108000
1	0.594489000	7.666623000	5.038716000
5	-0.264409000	6.741384000	4.391468000
1	-1.031913000	7.427039000	3.804776000
1	0.594668000	6.232110000	3.727813000
3	1.952143000	4.685688000	4.102546000
1,2-Li[B₄H₁₁]* MeCN E = -140.110009587 Ha			
1	0.236793000	6.452356000	4.557331000
5	0.111383000	5.454762000	5.280981000
1	-0.879906000	7.717023000	5.806959000
5	0.096328000	7.069040000	6.002407000
1	0.077283000	6.941625000	7.397055000
5	0.062477000	5.705666000	7.076245000
1	1.032210000	5.259353000	7.631351000
1	1.036775000	4.760000000	4.982924000
1	-0.985847000	5.308031000	7.482311000
3	2.493637000	5.219360000	6.377136000
1	1.015448000	7.918002000	5.840125000
5	2.353890000	7.575966000	5.962250000
1	2.602102000	6.778515000	5.097741000
1	2.695864000	8.691955000	5.712962000
1	2.539274000	7.221649000	7.093422000
1	-1.056380000	5.174815000	4.905903000
5	-1.328544000	3.828769000	4.816030000
1	-0.807727000	3.183750000	5.679255000
1	-2.499616000	4.044563000	4.995388000
1	-0.191070000	3.549067000	3.691403000
{1,2-Li[B₄H₁₁]}* MeCN E = -139.374237706 Ha			
1	0.147247000	6.596571000	4.414960000
5	0.326457000	5.397057000	4.772691000
1	-1.053755000	7.401449000	5.710888000
5	-0.005771000	6.850692000	5.790466000
1	-0.227244000	6.255847000	7.043954000
5	0.086907000	5.177591000	6.462762000
1	0.977373000	4.652591000	7.042679000
1	1.356987000	4.997840000	4.342474000
3	2.830452000	5.198420000	5.908912000
1	0.808308000	7.758657000	6.025532000
5	2.200218000	7.515755000	6.189032000
1	2.593400000	7.091722000	5.137738000
1	2.381770000	8.676944000	6.376270000
1	2.312380000	6.807569000	7.150357000

1	-0.636010000	4.968581000	4.097486000
5	-1.126436000	4.416972000	5.315782000
1	-1.009050000	6.429074000	6.718745000
1	-2.206763000	4.904929000	5.223040000
1	-0.994285000	3.2479	

1	-0.943328000	5.056478000	6.284465000
1	-0.373254000	5.874742000	4.528664000
5	-0.809951000	6.105548000	5.600600000
5	0.072382000	7.309726000	6.443927000
1	0.451196000	6.973810000	7.576878000
5	-0.060478000	5.657296000	7.196738000
1	0.905820000	4.962255000	7.148035000
1	-0.745889000	5.567638000	8.162172000
3	2.839638000	5.339529000	6.531293000
1	0.882653000	7.886628000	5.710735000
5	2.252629000	4.787905000	5.676912000
1	2.218133000	6.488818000	5.008767000
1	2.534707000	8.489566000	5.100659000
1	2.669456000	7.389017000	6.797976000
1	-0.632566000	8.235755000	6.880903000
5	-1.705831000	7.620266000	6.102775000
1	-2.040660000	6.355870000	5.575429000
1	-1.905697000	8.862910000	5.222907000
1	-2.444090000	7.580517000	7.034373000

cyc-Li[B₃H₄]⁺_MeCN E = -140.071745961 Ha			
1	-1.003832000	4.609484000	5.152135000
1	0.825554000	4.245515000	4.136472000
5	0.126436000	4.281627000	5.259920000
1	-1.251479000	7.513710000	6.400965000
5	-0.076097000	7.284959000	6.367723000
5	0.456458000	5.715069000	6.885441000
1	1.535335000	5.601678000	7.460960000
1	0.511476000	8.270229000	6.801415000
1	0.351806000	3.142772000	5.542806000
1	-0.345509000	5.059699000	7.495703000
1	0.983850000	4.990214000	5.872239000
5	0.660983000	5.244221000	3.328439000
1	-0.304139000	5.138951000	2.651769000
1	1.721768000	5.135384000	2.782025000
1	0.416126000	7.648948000	5.102388000
5	-0.112019000	7.135739000	4.069526000
1	-1.209592000	6.712100000	4.138647000
1	0.926460000	6.314269000	3.972070000
1	0.113653000	7.959714000	3.232560000
3	2.052795000	7.374520000	7.343383000

{cyc-Li[B₃H₃]⁺_MeCN E = -139.346349355 Ha			
1	-0.315426000	3.497985000	4.999311000
1	1.331287000	4.756479000	4.343355000
5	0.633354000	4.149014000	5.253098000
1	-0.278030000	8.173641000	6.934109000
5	0.277348000	7.336848000	6.298962000
5	-0.405479000	5.683025000	6.187530000
1	0.006692000	6.253595000	7.228752000
1	1.474022000	7.382445000	6.253738000
1	1.587745000	3.547007000	5.654657000
1	-1.450282000	5.237416000	6.516280000
1	0.606129000	4.877456000	6.326437000
5	5.503465000	5.385287000	3.561770000
1	-0.495620000	4.907473000	3.160522000
1	1.348749000	5.588698000	2.739453000
1	-0.029087000	7.890289000	5.004128000
5	-0.452793000	6.725975000	4.784576000
1	-1.528412000	6.904644000	4.326324000
1	0.517737000	6.633440000	3.925471000
3	2.934981000	6.488374000	7.265553000

BH₂_MeCN E = -25.2824014729 Ha			
5	4.045233000	-0.057097000	-0.137931000
1	3.990207000	-0.679466000	0.901242000

B⁺_MeCN E = -24.475216727 Ha			
5	4.045452000	-0.054616000	-0.142074000

st-B₂H₄_MeCN E = -52.0082422175 Ha			
5	1.479524000	-0.052117000	0.189496000
1	2.130325000	0.920693000	-0.045746000

1	-0.826044000	0.226421000	1.054747000
1	-0.732118000	-0.305571000	-0.896587000
5	-0.147035000	-0.042838000	0.110455000
1	2.092764000	-1.032884000	0.485210000

btf-B₂H₄_MeCN E = -52.0037086799 Ha			
5	1.539947000	-0.050275000	-0.262122000
1	2.583868000	-0.075934000	-0.785194000
1	0.683807000	-1.062309000	-0.449251000
1	-0.718707000	-0.342767000	1.037384000
5	0.266907000	-0.152279000	0.440530000
1	1.448010000	-0.352036000	1.039510000

B₂H₃⁺_MeCN E = -51.1723768703 Ha			
5	1.344948000	0.396037000	0.068575000
1	2.480539000	0.686496000	0.051753000
1	-0.894126000	0.172869000	1.079598000
1	-0.750126000	-0.490102000	-0.880159000
5	-0.276583000	-0.018713000	0.092598000

B₃H₄(μ₂H)₂(B₃H₇)⁺_MeCN E = -78.6702183073 Ha			
1	-0.922144000	5.292235000	5.151288000
5	-0.008280000	6.031689000	5.280040000
1	-0.568359000	7.285578000	5.409137000
5	0.315288000	7.236740000	6.359090000
1	-0.256984000	7.061114000	7.021160000
5	0.280193000	5.826466000	7.216531000
1	1.302702000	5.744717000	7.821715000
1	1.108353000	8.104437000	6.336291000
1	0.793324000	6.104174000	7.402323000
1	-0.5778437000	5.048057000	4.517480000

{B₃H₄(μ₂H)₂(B₃H₇)⁺_MeCN E = -77.8847125775 Ha			
1	-0.990693000	6.096589000	5.351911000
5	0.187964000	5.533591000	5.605176000
1	-0.582949000	8.103713000	5.688817000
5	-0.341882000	7.022247000	6.051506000
1	-0.516740000	6.881500000	7.361596000
5	0.535492000	6.112445000	7.101891000
1	1.318804000	6.128934000	7.964946000
1	0.563750000	4.875857000	4.719010000
1	0.183557000	4.875893000	6.759954000

B₃H₆(μ₂H)₂(B₃H₇)⁺_MeCN E = -78.6662241218 Ha			
1	-0.625283000	5.132884000	5.133500000
1	-0.035213000	7.006860000	4.650326000
5	0.277328000	5.897565000	5.286438000
1	-1.106519000	7.850855000	6.144704000
5	-0.003794000	7.483390000	5.877066000
1	0.344837000	6.936810000	7.950498000
5	0.404315000	6.002199000	7.026262000
1	0.675273000	5.270544000	7.257530000
1	0.880058000	8.282674000	5.925687000
1	1.360832000	5.566335000	4.913736000

{B₃H₅(μ₂H)₂(B₃H₇)⁺_MeCN E = -77.8847177194 Ha			
1	0.429852000	5.488346000	4.682004000
5	0.320623000	6.050622000	5.697222000
1	-0.800215000	8.415164000	6.295238000
5	-0.243831000	7.401246000	6.441547000
1	0.061462000	7.170910000	7.714211000
5	-0.239829000	5.965289000	7.239622000
1	0.815025000	5.351442000	6.714961000
1	0.815863000	7.283951000	5.649043000
1	-0.790331000	5.303389000	8.025769000

B₂H₅(BH₂)₂(B₃H₇)⁺_MeCN E = -78.656376258 Ha			
5	1.488154000	0.007770000	0.108627000
1	2.142361000	0.300418000	-0.848743000
1	0.627604000	-0.926767000	-0.272412000
1	-0.952710000	-0.229434000	0.790464000
1	-0.683267000	0.350499000	-1.168265000
1	0.599445000	0.976462000	0.285006000
5	-0.232355000	0.047316000	-0.112437000

5	2.348506000	-0.382557000	1.476148000
1	2.692900000	0.442144000	2.266889000
1	2.732905000	-1.492963000	1.684875000

{B₂H₄(BH₂)₂(B₃H₇)⁺_MeCN E = -77.8653285569 Ha			
5	1.314273000	-0.076921000	0.406876000
1	1.590600000	0.213389000	-0.855616000
1	0.363115000	-0.937697000	0.027903000
1	-0.527558000	0.423758000	-1.444011000
1	0.413888000	0.923868000	0.465625000
5	0.268018000	0.209276000	-0.628658000
5	2.486698000	-0.400864000	1.549738000
1	2.797102000	0.427918000	2.332827000
1	3.010115000	-1.460406000	1.565002000

arachno-B₄H₁₀_MeCN E = -104.517592389 Ha			
5	-1.931890000	2.174843000	6.147719000
5	-2.447555000	0.679494000	6.666631000
5	-0.805996000	0.761921000	6.399425000
5	-0.410904000	2.034903000	5.163253000
1	-2.233985000	3.114050000	6.781723000
1	-3.036902000	1.463028000	5.792567000
1	-3.124018000	0.295188000	7.536802000
1	-1.688517000	-0.227978000	6.096058000
1	-0.087214000	0.424110000	7.262276000
1	-0.262442000	0.716523000	5.212175000
1	0.256492000	2.697319000	5.895653000
1	-0.119499000	2.062158000	4.012719000
1	-1.644295000	2.448382000	4.902432000

arachno-B₄H₉⁺_MeCN E = -104.532528181 Ha			
5	-1.727224000	2.383672000	6.540227000
5	-2.505379000	0.856037000	6.224733000
5	-0.807653000	0.891130000	6.620661000
5	-1.258269000	1.561015000	5.076760000
1	-1.441968000	3.185398000	7.346239000
1	-2.975143000	2.109916000	6.614261000
1	-2.378697000	0.859158000	4.896304000
1	-3.505106000	0.243156000	6.342916000
1	-1.616740000	-0.092813000	6.737468000
1	-0.000925000	0.854057000	7.469970000
1	-0.263032000	0.670995000	5.484853000
1	-0.916954000	1.712409000	3.959165000
1	-1.621053000	2.879765000	5.366482000

bis-B₄H₁₀_MeCN E = -105.308987052 Ha			
5	1.526144000	0.027208000	0.025687000
1	2.111549000	0.321298000	-0.970905000
1	0.655542000	-0.917064000	-0.287790000
1	-0.864359000	-0.236327000	0.862798000
1	-0.739097000	0.337624000	-1.114678000
1	0.639255000	0.978668000	0.260790000
5	-0.213245000	0.045914000	-0.091056000
5	2.317118000	-0.381311000	1.466680000
1	1.731716000	-0.675407000	2.463272000
1	3.187714000	0.562965000	1.780160000
1	3.204014000	-1.332764000	1.231575000
5	4.056508000	-0.400060000	1.583422000
1	4.582364000	-0.691714000	2.607041000
1	4.707618000	-0.117757000	0.629567000

bis-B₄H₉⁺_MeCN E = -104.524294050 Ha			
5	1.489924000	0.116606000	-0.183696000
1	1.955859000	0.460038000	-1.216872000
1	0.689277000	-0.88	

5	1.979844000	-0.911314000	1.967222000
1	3.753434000	0.775627000	1.401406000
1	3.167008000	-0.991919000	2.269994000
5	3.267534000	-0.211778000	0.971635000
1	3.806670000	-1.000335000	0.340631000
1	1.382638000	-0.389699000	2.974965000
5	0.866984000	-1.649855000	3.027606000
1	-0.277091000	-1.578627000	2.750669000
1	1.529661000	-2.112208000	1.931213000
1	1.289347000	-2.192556000	3.983368000

n-bis-B₄H₁₀(BH₂)⁺ MeCN E = -131.917406720 Ha			
5	1.436526000	-0.030588000	0.029472000
1	2.004619000	0.138235000	-1.004379000
1	0.502094000	-0.939706000	-0.171942000
1	-0.924803000	-0.066845000	0.973723000
1	-0.847330000	0.328540000	-1.050513000
1	0.624760000	0.993457000	0.210664000
5	-0.300313000	0.090745000	-0.024780000
5	2.251504000	-0.365237000	1.474133000
1	1.718471000	-0.513674000	2.527291000
1	3.223002000	0.507702000	1.684130000
1	3.033102000	-1.430908000	1.318874000
5	3.977949000	-0.557199000	1.488297000
1	4.647055000	-0.741041000	2.438997000
1	4.474313000	-0.117133000	0.412181000
5	5.147941000	-1.177277000	-0.120700000
1	6.265047000	-0.761379000	-0.018968000
1	4.937785000	-2.196364000	0.480116000
1	4.628279000	-1.113863000	-1.198591000

n-bis-B₄H₁₀(BH₂)⁺ MeCN E = -131.144884304 Ha			
5	1.485970000	-0.095051000	0.075467000
1	2.189640000	-0.168041000	-0.878302000
1	0.433335000	-0.847124000	-0.127800000
1	-0.896280000	0.401481000	0.779710000
1	-0.584103000	0.527358000	-1.260457000
1	0.888579000	1.070861000	0.060553000
5	-0.182549000	0.325782000	-0.164390000
5	2.049920000	-0.389396000	1.643517000
1	1.451339000	-0.279876000	2.657543000
1	3.246124000	0.288777000	1.841630000
1	2.635022000	-1.643225000	1.687071000
5	3.637042000	-0.909807000	1.935972000
1	4.559119000	-1.138431000	1.082813000
1	4.150514000	-1.167759000	3.074848000
5	5.202470000	-1.460584000	2.249671000
1	5.353091000	-2.626734000	2.262164000
1	6.032333000	-0.647894000	2.432142000

Li₂BH MeCN E = -40.3932025845 Ha			
5	4.045452000	-0.054616000	-0.142074000
1	3.989988000	-0.681947000	0.905385000
3	2.597968000	0.390187000	-1.812668000
3	5.721953000	1.107899000	-1.131207000

{Li₂B}⁺ MeCN E = -39.6615849955 Ha			
5	1.663657000	-0.528289000	-1.065902000
3	1.379564000	-2.708605000	-0.347846000
3	1.978928000	1.675406000	-1.694124000

Li₂[B₂H₄] MeCN E = -67.1751644909 Ha			
5	0.023394000	0.078419000	-0.062958000
5	1.419259000	-0.095271000	-0.799200000
1	1.581650000	-0.367921000	-1.976733000
1	-0.138968000	0.350822000	1.114638000
3	-0.236255000	-0.382875000	-2.159560000
3	1.678842000	0.365675000	1.297675000
1	-1.078253000	-0.035095000	-0.573698000
1	2.520804000	0.018688000	-0.288507000

{Li₂[B₂H₄]}⁺ MeCN E = -66.4127187897 Ha			
5	0.018754000	0.092469000	-0.000562000

5	1.440455000	-0.024740000	-0.516940000
1	-0.465134000	-0.762709000	0.695607000
3	-0.123395000	-1.041569000	-2.125028000
3	1.444544000	1.113177000	1.662319000
1	-0.671694000	1.039560000	-0.268774000
1	2.545293000	-0.115250000	-0.918233000

Li₂[B₂H₇] conf0 MeCN E = -93.8450241019 Ha			
1	-0.598376000	5.398842000	4.672642000
3	-1.087153000	7.193352000	4.237502000
5	0.337615000	5.856937000	5.307700000
1	-0.773746000	8.107591000	5.936011000
5	0.193326000	7.383550000	6.099652000
1	-0.085749000	7.041620000	7.381182000
5	0.196350000	5.764556000	7.027592000
1	1.194221000	5.607998000	7.717307000
1	1.207537000	8.036537000	6.271585000
1	1.396809000	5.580252000	4.758093000
1	-0.778680000	5.230777000	7.491543000
3	2.270767000	6.263539000	6.204147000

{Li₂[B₂H₇]}⁺ conf0 MeCN E = -93.0887188017 Ha			
1	-0.440439000	5.533680000	4.328178000
3	-0.858091000	7.525929000	3.976678000
5	0.344202000	5.905652000	5.169858000
1	-1.203951000	7.698214000	6.091704000
5	-0.205048000	7.043917000	6.120602000
1	0.353404000	7.180588000	7.299291000
5	0.099035000	5.823498000	7.210960000
1	1.157909000	5.295404000	7.407125000
1	1.401552000	5.352499000	5.047572000
1	-0.744728000	5.568157000	8.014884000
3	2.361539000	6.501477000	6.166520000

Li₂[B₂H₇] conf1 MeCN E = -93.8328798254 Ha			
5	1.431915000	-0.403794000	0.080745000
1	2.071776000	-0.826597000	-0.875971000
1	-0.785454000	-1.339389000	0.318004000
1	-0.678151000	0.553946000	0.890229000
1	-0.861292000	1.109580000	-1.024369000
1	2.089053000	0.810620000	0.386184000
5	-0.308988000	-0.236398000	0.020466000
5	2.353495000	-0.041210000	1.368935000
1	1.856351000	0.431455000	2.380629000
1	3.543234000	-0.211227000	1.444394000
3	0.632902000	-0.331787000	-2.027536000
3	0.288817000	-0.796060000	1.998228000

{Li₂[B₂H₇]}⁺ conf1 MeCN E = -93.0866560984 Ha			
5	1.619649000	0.254534000	-0.386423000
1	2.395566000	0.166588000	-1.286904000
1	-0.546322000	0.017316000	0.810969000
1	-0.076554000	-1.443922000	-0.520157000
1	2.178663000	0.954469000	0.599310000
5	0.276481000	-0.440680000	0.060360000
5	1.943853000	-0.251296000	1.172520000
1	1.424567000	0.007973000	2.221219000
1	3.004304000	-0.793932000	1.275899000
3	0.348796000	-0.277640000	-2.239690000
3	-0.257194000	-1.028161000	2.362609000

/ln-Li₂[B₂H₁₀] MeCN E = -120.475768438 Ha			
1	-0.152985000	5.520715000	4.916804000
3	0.278262000	7.471780000	4.233579000
5	0.651809000	5.914207000	5.749568000
1	-0.614582000	8.015846000	6.097837000
5	0.379163000	7.436907000	6.496497000
1	-0.007200000	7.140759000	7.731206000
5	0.301059000	5.854323000	7.426223000
1	1.203086000	5.636332000	8.192602000
1	1.319517000	8.164730000	6.695239000
1	-0.759296000	5.364944000	7.782005000
3	-0.717022000	4.184895000	6.249274000

1	1.744226000	5.317121000	5.599388000
5	2.422540000	6.139550000	4.708864000
1	2.975546000	5.157804000	4.258511000
1	1.955261000	6.761648000	3.772025000
1	3.153036000	6.809685000	5.393170000

{/ln-Li₂[B₂H₁₀]}⁺ MeCN E = -119.771045221 Ha			
1	0.042679000	5.158211000	4.929251000
3	0.284252000	6.744487000	3.771373000
5	0.881279000	5.482788000	5.758549000
1	-0.322845000	7.618362000	5.779790000
5	0.610900000	7.082926000	6.297375000
1	0.482885000	7.152365000	7.597198000
5	0.401230000	5.805555000	7.474575000
1	1.275294000	5.461031000	8.207074000
1	1.674623000	7.832016000	6.919600000
1	-0.721168000	5.608478000	7.174509000
3	-1.396277000	4.790759000	6.246718000
1	1.708107000	6.444017000	5.937931000
5	2.059309000	6.824903000	5.364271000
1	2.069532000	7.359261000	4.281916000
1	3.127362000	6.564438000	5.818280000

cyc-Li₂[B₂H₁₀] MeCN E = -120.465182617 Ha			
1	-1.754587000	5.126155000	5.553130000
5	-0.677151000	5.127266000	4.986164000
1	-0.973567000	7.492759000	6.736281000
5	0.125207000	7.281526000	6.226681000
5	0.814951000	5.711290000	6.427766000
1	1.907042000	5.558213000	5.911697000
1	0.860247000	8.209645000	6.498239000
1	-0.557156000	4.097543000	4.330491000
1	0.825159000	5.236371000	7.558813000
1	0.135850000	4.662958000	5.945184000
1	-0.131948000	7.685368000	4.994288000
5	-0.254357000	6.617664000	4.223848000
1	-1.111962000	7.095314000	3.508482000
1	0.821622000	6.674381000	3.631843000
3	1.345502000	4.934997000	4.036898000
3	-1.194083000	5.777930000	7.418557000

{cyc-Li₂[B₂H₁₀]}⁺ MeCN E = -119.770486850 Ha			
1	-1.892019000	4.892784000	4.916305000
5	-0.774896000	5.118676000	4.577719000
1	-1.070863000	7.598525000	6.846886000
5	-0.029801000	7.384162000	6.271016000
5	0.246758000	5.611974000	6.049497000
1	0.869633000	8.118180000	6.546805000
1	-0.316895000	4.380392000	3.741381000
1	1.380581000	5.201774000	6.153516000
1	-0.520258000	5.018895000	6.759140000
1	-0.421357000	7.809533000	5.056027000
5	0.050799000	6.634891000	4.694683000
1	-0.942416000	6.295870000	3.919709000
1	1.037435000	6.788924000	4.040700000
3	1.597592000	4.657527000	4.341986000
3	-0.940566000	6.221760000	8.161293000

bis-Li₂[B₂H₁₀] MeCN E = -120.453322607 Ha			
5	1.407686000	-0.486645000	0.017197000
1	1.536275000	-1.228474000	-0.934454000
1	0.049197000	-0.463859000	0.119561000
1	-0.043480000	1.526039000	0.549721000
1	-0.408376000	0.838947000	-1.346517000
1	1.459042000	0.740782000	-0.557017000
5	0.191603000	0.737467000	

1	1.986782000	-2.495448000	0.957166000
1	0.789978000	-4.060567000	0.531979000
{tr-BB-Li₂[B₄H₉]}* MeCN E = -119.770486850 Ha			
1	-1.892019000	4.892784000	4.916305000
5	-0.774896000	5.118676000	4.577719000
1	-1.070863000	7.595825000	6.846886000
5	-0.029801000	7.384162000	6.271016000
5	0.246758000	5.611974000	6.049497000
1	0.869633000	4.118180000	6.546805000
1	-0.316895000	8.380392000	3.741381000
1	1.380581000	5.201774000	6.153516000
1	-0.520258000	5.018895000	6.759140000
1	-0.421357000	7.809533000	5.056027000
5	0.050799000	6.634891000	4.694683000
1	-0.942416000	6.295870000	3.919709000
1	1.037435000	6.788924000	4.040700000
3	1.597592000	4.657527000	4.341986000
3	-0.940566000	6.221760000	8.161293000
lin-BB-Li₂[B₄H₁₀] MeCN E = -120.419380287 Ha			
5	4.732299000	1.772503000	22.241243000
1	2.345008000	2.342573000	22.268705000
5	2.806089000	1.475664000	22.945468000
1	2.205409000	0.443755000	22.903973000
1	3.987972000	0.869856000	22.753358000
1	5.652820000	3.018804000	24.202622000
5	5.693606000	2.733893000	23.024543000
1	4.741863000	1.505914000	21.058027000
1	6.612083000	3.325254000	22.483749000
1	2.829389000	2.102600000	24.065771000
5	3.015433000	1.299837000	25.123146000
1	3.617051000	0.276731000	24.905804000
1	1.925210000	1.119442000	25.578121000
1	3.681550000	2.121443000	25.711671000
3	5.377674000	1.169059000	24.652707000
3	5.698231000	3.152339000	20.838447000
{lin-BB-Li₂[B₄H₉]}* MeCN E = -119.77275153 Ha			
5	4.415735000	0.988610000	23.432450000
1	3.796467000	3.420100000	23.275040000
5	3.252223000	2.216265000	23.214520000
1	2.643197000	2.111774000	22.195637000
1	4.344026000	0.179443000	22.538313000
1	5.572942000	3.147265000	24.028249000
5	4.925942000	2.710708000	23.114883000
1	5.317656000	3.073056000	22.036319000
1	2.420291000	2.351614000	24.210933000
5	2.989442000	1.166623000	24.567293000
1	5.247696000	0.637247000	24.222618000
1	2.078411000	0.401443000	24.536501000
1	3.369845000	1.468246000	25.671936000
3	5.268218000	1.923407000	25.550498000
3	4.537732000	1.428853000	21.104138000
1,1-Li₂[B₅H₁₃] MeCN E = -147.107011882 Ha			
3	1.563450000	8.225417000	4.944250000
5	0.865754000	5.936767000	5.727214000
1	-0.976507000	7.536541000	5.950167000
5	0.105934000	7.308739000	6.423977000
1	-0.206489000	6.931885000	7.664523000
5	0.342214000	5.757386000	7.351403000
1	1.254072000	5.688082000	8.133493000
1	1.750071000	8.301837000	6.698261000
1	-0.603046000	5.044258000	7.623446000
3	0.162755000	3.656581000	6.517084000
1	2.044433000	5.495428000	5.749978000
5	2.779942000	6.387865000	5.042633000
1	3.654120000	5.644480000	4.953631000
1	2.405314000	6.733675000	3.944457000
1	3.096197000	7.308127000	5.765118000

1	0.290532000	5.820114000	4.613820000
5	0.016151000	4.499018000	4.483058000
1	-1.019622000	4.246349000	5.059091000
1	-0.156816000	4.674865000	3.304101000
1	0.891938000	3.684437000	4.670472000
{1,1-Li₂[B₅H₁₃]}* MeCN E = -146.377673768 Ha			
3	1.934708000	8.579000000	5.571074000
5	0.847077000	6.140845000	5.285244000
1	-0.955323000	7.655690000	5.885120000
5	0.090078000	7.258125000	6.316442000
1	-0.388444000	6.461879000	7.310113000
5	0.211210000	5.446371000	6.729915000
1	1.215360000	5.176382000	7.337870000
1	0.713290000	8.044189000	6.991415000
1	-0.681854000	4.632584000	6.864970000
3	0.500416000	3.637885000	8.320086000
1	1.983309000	5.592540000	5.180823000
5	2.835076000	6.593785000	4.910017000
1	3.643757000	5.805401000	4.509531000
1	2.504031000	7.380208000	4.057047000
1	3.138930000	7.089101000	5.965370000
1	0.235664000	5.936470000	4.207197000
5	-0.242969000	4.837446000	5.002262000
1	-1.403043000	5.063827000	4.849203000
1	0.187187000	3.785654000	4.651838000
1,2-Li₂[B₅H₁₃] MeCN E = -147.100994834 Ha			
1	-0.431266000	6.146053000	5.116994000
3	1.534727000	8.273482000	5.120639000
5	0.525869000	6.156303000	5.855929000
5	0.700221000	7.390236000	7.010480000
1	0.649901000	6.675320000	8.187455000
5	0.457675000	5.625639000	7.488251000
1	1.387401000	5.009510000	7.931716000
1	1.702385000	8.043399000	7.155863000
1	-0.616181000	5.330755000	7.979877000
3	-1.295768000	4.847464000	6.219176000
1	1.467981000	5.428667000	5.406156000
5	2.167818000	6.217067000	4.559021000
1	2.639790000	5.246948000	4.022424000
1	1.579449000	6.898249000	3.747491000
1	2.995762000	6.835370000	5.191101000
1	-0.304433000	8.089060000	7.399862000
5	-0.857027000	8.809587000	6.417972000
1	-1.756425000	8.139673000	5.990734000
1	-1.193511000	9.679396000	7.182973000
1	-0.114081000	9.246897000	5.570625000
{1,2-Li₂[B₅H₁₃]}* MeCN E = -146.389402596 Ha			
1	-0.574699000	6.210984000	5.398319000
3	1.650668000	8.767275000	4.209511000
5	0.401497000	6.476136000	6.030937000
5	0.878338000	7.315907000	7.435802000
1	0.386431000	6.726000000	8.514061000
5	0.222356000	5.712562000	7.665758000
1	0.983652000	4.876972000	8.041892000
1	2.045016000	7.470339000	7.555137000
1	-0.948939000	5.503562000	7.871396000
3	-1.412211000	4.665831000	6.213527000
1	1.450997000	5.910883000	5.577560000
5	1.948001000	6.511204000	4.494658000
1	2.472179000	5.506546000	4.104389000
1	1.144658000	6.943260000	3.704381000
1	2.736437000	7.326446000	4.917544000
1	0.239721000	8.443299000	7.572970000
5	-0.011855000	8.232580000	6.260655000
1	-1.199583000	8.317287000	6.241200000
1	0.584048000	9.144543000	5.754306000
bis-Li₂[B₅H₁₃] MeCN E = -147.090545340 Ha			
5	1.342521000	-0.533275000	-0.010470000

1	1.354057000	-1.325672000	-0.926526000
1	0.005394000	-0.371902000	0.150630000
1	0.140263000	1.628850000	0.516993000
1	-0.382852000	0.920597000	-1.340582000
1	1.503141000	0.659807000	-0.622653000
5	0.248899000	0.798681000	-0.341987000
5	2.248443000	-0.633829000	1.463087000
1	1.533909000	-1.221049000	2.295567000
1	2.378486000	0.531052000	1.871876000
1	4.032661000	-2.518972000	1.272957000
5	3.836446000	-1.353933000	1.606821000
1	4.338372000	-1.193437000	2.696748000
1	4.878228000	-0.709372000	1.003087000
5	4.801177000	-0.370577000	-0.238389000
1	4.325793000	0.738509000	-0.279707000
1	5.988056000	-0.395558000	-0.483250000
1	4.226025000	-1.147908000	-0.975294000
3	0.621837000	0.491188000	2.413919000
3	2.917997000	-2.222275000	-0.169948000
{bis-Li₂[B₅H₁₃]}* conf0 MeCN E = -146.349686684 Ha			
5	1.287184000	-0.368375000	-0.126196000
1	1.393372000	-0.952747000	-1.172396000
1	-0.043604000	-0.312828000	0.027201000
1	0.019926000	1.545354000	0.901867000
1	-0.447812000	1.324132000	-1.082552000
1	1.436319000	0.917848000	-0.434715000
5	0.164089000	0.961701000	-0.135125000
5	2.154465000	-0.816542000	1.272929000
1	1.553469000	-1.290241000	2.215778000
1	2.808732000	0.230105000	1.775209000
5	3.747380000	-0.776907000	1.493358000
1	4.342887000	-1.062609000	2.481655000
1	4.499268000	0.045292000	0.818459000
5	4.876816000	-0.718453000	-0.187610000
1	4.103767000	-0.536880000	-1.098365000
1	5.930558000	-0.167263000	-0.327840000
1	5.023340000	-1.878896000	1.319366000
3	0.391878000	0.257189000	2.547411000
3	3.064159000	-2.109882000	-0.471077000
bis-Li₂[B₅H₁₃] MeCN E = -147.076094452 Ha			
5	1.454720000	-0.423326000	0.371434000
1	2.118837000	-1.091904000	-0.385228000
1	0.171394000	-0.798947000	0.246262000
1	-0.702633000	0.999585000	0.097622000
1	-0.073280000	0.087966000	-1.611106000
1	1.268969000	0.785003000	-0.193892000
5	0.091104000	0.301684000	-0.404925000
5	1.894846000	-0.283308000	-0.004828000
1	1.240370000	0.491144000	2.670600000
1	3.041551000	0.282084000	1.927196000
1	1.903537000	-1.380264000	2.537029000
5	4.295077000	-0.150630000	2.415332000
1	4.781615000	0.943581000	2.239756000
1	4.087707000	-0.301495000	3.615098000
5	4.930152000	-1.452676000	1.448691000
1	4.404111000	-2.573802000	1.613640000
1	4.820843000	-1.216321000	0.249066000
1	6.124807000	-1.594158000	1.707544000
3	3.548576000	-2.069641000	3.137868000
3	1.432905000	-1.046477000	-2.187372000
{bis-Li₂[B₅H₁₃]}* conf1 MeCN E = -146.394134705 Ha			
1	1.888422000	-0.498912000	0.217432000
1	2.192557000	-0.895974000	-0.877000000
1	0.573782000	-0.684189000	0.313039000
1	0.168152000	1.071205000	1.224873000
1	0.041172000	0.910504000	-0.832793000
1	1.837782000	0.828751000	0.116050000
5	0.553327000	0.616238000	0.196732000

5	2.634268000	-1.053198000	1.656198000
1	2.037123000	-0.622746000	2.622760000
1	2.4866640		

3	3.709426000	-0.239802000	22.653414000
1	1.877671000	1.653375000	23.705948000
5	1.476243000	2.934438000	24.176300000
1	0.431907000	2.440007000	24.515377000
1	2.060857000	3.403581000	25.129306000
1	1.371023000	3.692218000	23.243974000
{pinc-BB-Li₂[B₅H₁₂]}*_{MeCN} E = -146.350526975 Ha			
5	4.632080000	2.077121000	22.952636000
1	5.513891000	1.315295000	22.645166000
5	3.230910000	1.498082000	23.681933000
1	5.232245000	3.073735000	23.608438000
5	5.047792000	3.695962000	22.474183000
1	4.314807000	4.622652000	22.649152000
1	4.349351000	2.779130000	21.858375000
1	6.076118000	3.898165000	21.923904000
1	3.466131000	0.993598000	24.865454000
5	2.816179000	-0.001006000	24.107176000
1	1.774667000	-0.266062000	24.625832000
1	3.605346000	-0.917362000	24.032549000
3	3.243632000	5.128107000	24.254570000
3	4.213465000	-0.262971000	22.293575000
1	2.139731000	2.168482000	23.666928000
5	2.122075000	3.119198000	24.599473000
1	1.274707000	2.691382000	25.330169000
1	3.147772000	3.398865000	25.172077000
1	1.722513000	3.998067000	23.862042000
1,7-BB-Li₂[B₅H₁₃]*_{MeCN} E = -147.048318143 Ha			
5	4.159268000	2.159078000	22.539658000
1	3.730317000	2.655381000	21.522593000
5	3.236040000	1.828951000	23.766240000
1	5.349575000	1.956309000	22.544823000
1	3.678523000	1.749640000	24.954772000
5	3.774221000	0.390044000	25.076529000
1	2.981472000	-0.424040000	24.698072000
1	3.785035000	0.478475000	26.271222000
3	3.269444000	4.193874000	23.630980000
3	3.425256000	-0.280583000	22.743036000
1	1.989775000	1.637299000	23.751420000
5	1.511445000	2.892858000	24.108532000
1	0.449138000	2.392006000	24.368652000
1	1.968140000	3.482337000	25.060831000
1	1.464395000	3.562569000	23.099794000
1	4.999484000	0.340665000	24.705473000
1	5.124269000	-1.699304000	25.243311000
5	5.418062000	-0.902254000	24.400916000
1	5.043602000	-1.173022000	23.282164000
1	6.565114000	-0.541744000	24.415604000
{1,1-BB-Li₂[B₅H₁₂]}*_{MeCN} E = -146.388560990 Ha			
5	4.657783000	1.789222000	23.235889000
1	4.359755000	1.857293000	22.071373000
5	3.456675000	1.586109000	24.546090000
1	5.461739000	2.615441000	23.566549000
1	3.631302000	2.430386000	25.371265000
5	4.096422000	0.293758000	25.697296000
1	3.354115000	-0.527072000	26.134926000
1	4.880849000	0.810210000	26.428782000
3	3.825304000	3.926872000	24.131817000
3	2.868877000	0.636373000	21.797498000
1	2.228359000	1.279363000	24.424466000
5	1.595732000	2.170963000	23.627939000
1	0.605913000	2.160939000	24.304207000
1	2.032330000	3.278226000	23.455103000
1	1.438579000	1.564252000	22.593987000
1	4.958150000	-0.420007000	24.892598000
1	3.702137000	-0.527781000	23.308933000
5	4.326732000	0.356560000	23.981415000
1	5.398221000	0.684058000	23.332322000

tr-BB-Li₂[B₅H₁₃]*_{MeCN} E = -147.049098383 Ha

5	4.597511000	2.684046000	22.260436000
1	2.585580000	3.221035000	23.526144000
5	2.842803000	2.099057000	23.182884000
1	1.920215000	1.540934000	22.670858000
1	3.698527000	1.765739000	22.216537000
1	6.135382000	2.010369000	24.152093000
5	5.847183000	2.676626000	23.188241000
1	4.343995000	3.443158000	21.364984000
1	3.254091000	1.645342000	24.308650000
5	3.371489000	0.305023000	24.334613000
1	3.583442000	-0.213608000	23.266788000
1	2.378201000	-0.084905000	24.870768000
1	4.348886000	0.342804000	25.047446000
3	4.413285000	4.594986000	23.526138000
3	5.541511000	0.407937000	23.218965000
1	6.885617000	3.296505000	22.778471000
5	6.718235000	4.525497000	23.365433000
1	6.131564000	5.210167000	22.557689000
1	7.903334000	4.729150000	23.384501000
1	6.244968000	4.582089000	24.479316000
{tr-BB-Li₂[B₅H₁₂]}*_{MeCN} E = -146.394727865 Ha			
5	4.494180000	1.776920000	22.937446000
1	4.007797000	2.446086000	25.395165000
5	3.459106000	2.343400000	24.325713000
1	2.919766000	3.357344000	23.969186000
1	4.069169000	2.115208000	21.851087000
1	6.563218000	2.258790000	24.378463000
5	5.846415000	2.663077000	23.503435000
1	2.442637000	1.537268000	24.518390000
5	3.216937000	0.735254000	23.766532000
1	4.965158000	0.661662000	22.812561000
1	2.472183000	0.345698000	22.926965000
1	3.616552000	-0.104697000	24.534971000
3	3.591863000	3.867510000	22.132307000
3	5.288782000	0.798924000	25.072806000
1	6.661369000	2.979193000	22.488061000
5	6.297894000	4.188601000	22.798616000
1	5.574548000	4.612690000	21.943173000
1	7.256927000	4.815269000	23.100500000
1	5.630322000	3.941167000	23.880596000

Li[B₂H₄]*_{MeCN} E = -58.9679475224 Ha

5	1.010776000	0.581857000	0.183087000
1	2.061948000	0.828907000	0.653333000
1	0.156107000	-0.118563000	0.931660000
1	-1.396264000	-0.167647000	-0.551191000
5	-0.310679000	0.196364000	-0.275917000
3	1.283700000	-0.949797000	-1.608079000

{Li[B₂H₄]}*_{MeCN} E = -58.1577370651 Ha

5	0.470962000	-0.169663000	0.582776000
1	1.383934000	-0.372349000	1.281216000
1	-1.666757000	0.316882000	-0.982432000
5	-0.735299000	0.103667000	-0.312031000
3	1.290798000	-0.336524000	-1.889967000

Li[B₃H₆]*_{MeCN} E = -85.6400986607 Ha

3	-0.410496000	5.496016000	4.312095000
3	-0.922692000	7.441223000	4.021669000
5	0.360716000	5.925206000	5.153742000
1	-1.196487000	7.718040000	6.146101000
5	-0.203302000	7.047555000	6.113290000
1	0.444096000	7.151149000	7.257049000
5	0.082826000	5.824653000	7.200029000
1	1.081681000	5.201528000	7.380382000
1	1.460233000	5.466764000	5.079416000
1	-0.792731000	5.655404000	8.003080000

{Li[B₃H₆]}*_{MeCN} E = -84.8979332547 Ha

3	-0.073352000	5.714410000	4.050090000
1	-1.099816000	7.665105000	3.929562000
5	0.184632000	5.885056000	5.187461000

1	-1.112690000	7.845875000	6.114265000
5	-0.344151000	6.959873000	6.232837000
1	0.096219000	6.941709000	7.384105000
5	0.686614000	5.850229000	6.685580000
1	1.341140000	5.355553000	7.526076000
1	1.017979000	5.054323000	5.553798000

Li[B₃H₆]*_{conf1} MeCN E = -85.6314444486 Ha

5	1.637591000	6.160933000	5.708224000
1	0.772900000	6.711055000	6.293639000
5	3.049320000	7.001684000	5.115361000
1	2.665480000	7.918970000	4.432675000
1	3.571685000	7.385812000	6.158986000
1	3.884280000	6.372489000	4.462697000
5	2.422631000	4.973834000	5.060725000
1	3.248787000	4.366568000	5.704298000
1	2.290100000	4.620010000	3.926840000
3	4.670992000	5.792705000	6.097686000

{Li[B₃H₆]}*_{conf1} MeCN E = -84.8973460108 Ha

5	1.856646000	6.036679000	5.636009000
1	0.973391000	6.425245000	6.300799000
5	3.147293000	6.844960000	5.124825000
1	3.427443000	7.963745000	5.333144000
1	3.986307000	6.274451000	4.425024000
5	2.975289000	5.309905000	4.786330000
1	3.376043000	4.340146000	4.265340000
1	1.723102000	4.850413000	5.328194000
3	4.082772000	5.339546000	7.338077000

arachno-Li[B₄H₈]*_{MeCN} E = -112.321268918 Ha

5	-1.931323000	2.287729000	6.562652000
5	-2.691138000	0.618156000	6.616904000
5	-1.006785000	0.890745000	6.277133000
5	-0.818154000	2.166191000	5.108747000
1	-1.554599000	2.815995000	5.710590000
1	-2.839573000	2.912300000	6.079048000
1	-3.516327000	0.496328000	5.739705000
1	-2.993243000	0.094843000	7.646447000
1	-1.744995000	-0.195633000	6.116762000
1	-0.170266000	0.669075000	7.087550000
1	-0.452575000	0.872665000	5.057306000
1	0.220939000	2.751592000	5.088471000
1	-1.454168000	2.201030000	4.079593000
3	-3.288327000	2.010948000	4.585063000

{arachno-Li[B₄H₈]}*_{MeCN} E = -111.557750718 Ha

5	-2.017995000	2.200995000	6.147800000
5	-2.705804000	0.613140000	6.044610000
5	-0.994985000	0.858166000	6.476600000
5	-0.497973000	2.227522000	5.605695000
1	-2.495894000	3.157149000	6.663728000
1	-1.570474000	2.502256000	4.893303000
1	-3.117744000	0.473950000	4.934539000
1	-3.385981000	0.187218000	6.940761000
1	-1.673646000	-0.201160000	5.996719000
1	-0.448866000	0.504588000	7.459356000
1	-0.148339000	0.959201000	5.428380000
1	0.428605000	2.926232000	5.438997000
3	-4.157249000	1.981635000	7.495171000

bis-Li[B₄H₈]*_{conf0} MeCN E = -112.279585850 Ha

5

5	4.906265000	1.968422000	23.273370000
1	4.914631000	0.613471000	21.192223000
1	3.082233000	2.648326000	24.818006000
5	2.234420000	1.647440000	24.676246000
1	1.132181000	2.058790000	24.826062000
1	2.633692000	0.723648000	25.305622000
3	7.507322000	2.138337000	23.236639000

lin-1-BBB-Li[B₅H₁₂]_{conf1} MeCN E = -112.263000179 Ha			
5	3.972868000	2.251108000	22.302927000
1	3.478345000	2.674874000	21.305790000
5	3.429932000	1.837214000	23.717615000
1	5.285054000	2.473356000	22.294640000
5	4.862420000	3.210919000	23.341232000
1	5.485570000	2.887117000	24.299421000
1	4.949380000	4.384773000	23.057553000
1	3.795406000	1.285376000	24.698824000
3	2.927720000	4.552554000	22.849720000
1	2.141242000	1.914142000	23.676655000
5	1.711466000	3.053869000	24.230407000
1	0.842992000	2.594293000	24.913706000
1	2.522483000	3.705585000	24.839729000
1	1.291313000	3.604378000	23.232389000

{lin-1-BBB-Li[B₅H₁₂]_{conf1} MeCN E = -111.551730638 Ha			
5	4.649341000	2.542068000	22.625102000
1	3.554361000	2.153798000	21.986257000
5	3.236176000	1.837798000	23.265454000
1	5.589110000	2.280535000	21.970098000
5	4.174518000	3.004419000	24.099881000
1	4.916539000	3.214740000	24.991352000
1	4.521980000	3.781755000	22.997089000
3	3.119591000	0.675416000	23.431374000
3	2.016847000	4.949496000	22.039008000
1	1.990417000	2.352008000	23.214340000
5	2.432831000	3.082956000	24.230055000
1	1.872007000	2.661766000	25.191386000
1	2.099990000	4.183285000	23.879483000

lin-3-BBB-Li[B₅H₁₂]_{conf1} MeCN E = -112.254230537 Ha			
5	4.545135000	1.704918000	22.111269000
1	2.192799000	2.415374000	22.721008000
5	3.285648000	2.145623000	23.101890000
1	3.632291000	0.922949000	22.751299000
1	5.579733000	2.774325000	24.181133000
5	5.321712000	2.753557000	23.005751000
1	4.388557000	1.501482000	20.953936000
1	5.730169000	3.703742000	22.399940000
1	3.465901000	2.039766000	24.323798000
5	3.092343000	1.317480000	25.112166000
1	4.118709000	0.694310000	25.254734000
1	2.167971000	0.677847000	24.707909000
1	2.849660000	2.063913000	26.019156000
3	5.841767000	0.803910000	24.172023000

{lin-3-BBB-Li[B₅H₁₂]_{conf1} MeCN E = -111.543096285 Ha			
5	3.936507000	1.347490000	22.444012000
1	1.841875000	2.762872000	23.474884000
5	2.969784000	2.489634000	23.293985000
1	2.717145000	1.258356000	22.330671000
5	4.512069000	2.778508000	23.203919000
1	4.494612000	0.900230000	21.503301000
1	5.571414000	3.275458000	23.176865000
1	3.613370000	3.658071000	23.343749000
5	4.044428000	1.373689000	24.272890000
1	5.110255000	1.567072000	24.787655000
1	4.198327000	0.399743000	23.421767000
1	3.150366000	1.001501000	24.978698000
3	4.472510000	0.286247000	26.402485000

commo-Li[B₅H₁₂] MeCN E = -138.955351626 Ha			
1	0.959081000	4.963173000	4.898041000
5	1.564823000	5.752043000	5.558442000

1	-0.488801000	7.032101000	5.525449000
5	0.464991000	7.036671000	6.239921000
1	-0.031340000	6.597273000	7.362166000
5	1.036603000	5.785231000	7.325526000
1	0.883455000	8.133267000	6.508223000
1	0.523486000	4.749281000	7.612146000
3	2.741066000	7.692972000	6.851016000
5	2.421759000	6.984978000	4.524343000
1	1.826756000	6.980844000	3.491963000
1	2.676732000	8.081556000	4.950122000
1	1.831234000	6.216100000	8.122339000
3	3.579779000	6.495418000	4.177541000
5	3.384141000	5.713947000	5.249495000
1	2.249632000	5.105873000	6.364883000
1	4.094316000	6.153488000	6.126357000
1	3.685498000	4.653473000	4.798626000

{commo-Li[B₅H₁₁]₁ MeCN E = -138.201001815 Ha			
1	1.055297000	4.419215000	4.997834000
5	1.518060000	5.340448000	5.577798000
1	-0.508262000	6.835793000	5.380087000
5	0.576657000	6.777916000	5.837910000
1	0.587836000	7.182585000	7.057399000
5	0.912893000	5.860323000	7.267554000
1	1.342599000	7.758970000	5.331788000
1	-0.059514000	5.347441000	7.712453000
3	3.387185000	7.309736000	8.105661000
5	1.885731000	6.766329000	4.642186000
1	1.578093000	6.848984000	3.507484000
1	1.832323000	5.980758000	8.023570000
1	3.076565000	7.156455000	4.801823000
5	3.272602000	5.880657000	5.350897000
1	2.483424000	5.029949000	6.291082000
1	3.897200000	6.273087000	6.299317000
1	3.887788000	5.259487000	4.551633000

lin-1-Li[B₅H₁₂] MeCN E = -138.944830882 Ha			
3	2.265897000	8.506977000	5.962898000
5	0.700732000	6.116040000	5.080372000
1	-0.985184000	7.706955000	5.804670000
5	0.039633000	7.284062000	6.250314000
1	-0.429681000	6.509177000	7.246381000
5	0.276245000	5.580849000	6.639927000
1	1.193713000	5.255893000	7.316597000
1	0.683925000	8.075791000	6.893600000
1	-0.637610000	4.653936000	6.641171000
1	1.886542000	5.641511000	4.929211000
5	2.810722000	6.586605000	4.885428000
1	3.588720000	5.899801000	4.282654000
1	2.532051000	7.588522000	4.270282000
1	3.149624000	6.781684000	6.032689000
1	0.207217000	6.413622000	4.043000000
5	-0.285309000	4.591789000	5.324656000
1	-1.349215000	4.770238000	4.810853000
1	0.220022000	3.516045000	5.214915000

{lin-1-Li[B₅H₁₁]₁ MeCN E = -138.200950997 Ha			
5	1.681296000	0.637327000	3.358161000
5	0.824996000	1.035903000	1.909833000
5	-0.138925000	0.263563000	3.132682000
5	-0.862418000	1.517517000	2.157020000
5	-1.170005000	1.583450000	3.922001000
1	2.474278000	-0.226398000	3.180566000
1	1.850713000	1.308177000	4.333425000
1	1.026725000	0.463683000	0.899294000
1	-0.538375000	-0.838069000	2.971362000
1	-1.626971000	1.259412000	1.298202000
1	-0.662832000	2.382277000	4.662553000
1	-2.266945000	1.246956000	4.214993000
1	1.900061000	1.571679000	2.368743000
1	0.169125000	2.184433000	1.663524000

1	-1.295157000	2.480428000	2.850928000
1	-0.128320000	0.599553000	4.327674000
3	1.276441000	3.219025000	4.769632000

lin-BBB-Li[B₅H₁₂] MeCN E = -138.943973204 Ha			
5	4.458396000	1.811442000	22.903891000
1	3.988112000	2.614890000	25.305540000
3	3.417416000	2.375886000	24.276645000
1	2.760887000	3.301921000	23.852662000
1	4.004602000	2.146484000	21.818425000
1	6.183222000	2.153100000	24.338107000
5	5.831651000	2.616281000	23.480260000
1	2.500468000	1.513042000	24.566049000
5	3.305624000	0.713393000	23.778214000
1	4.837188000	0.659712000	22.802952000
1	2.506556000	0.285044000	22.999568000
1	3.764862000	-0.063229000	24.565590000
3	3.657538000	3.888960000	22.220683000
1	6.677980000	2.995562000	22.477517000
5	6.319548000	4.176220000	22.832889000
1	5.611926000	4.650319000	21.985715000
1	7.278871000	4.792702000	23.165789000
1	5.646093000	3.908687000	23.892670000

{lin-BBB-Li[B₅H₁₁]₁ MeCN E = -138.174713418 Ha			
5	4.751271000	1.751880000	23.262753000
1	3.966111000	2.500098000	25.436443000
5	3.541988000	2.458662000	24.325636000
1	3.220378000	3.516505000	23.845752000
1	4.946579000	0.897131000	22.458156000
1	6.861193000	2.251494000	24.325917000
5	6.065585000	2.731739000	23.581136000
1	2.478070000	1.688854000	24.400455000
5	3.147466000	1.022279000	23.460557000
1	2.531852000	1.116449000	22.432600000
1	3.279496000	-0.074139000	23.899443000
3	1.794140000	3.081482000	22.368782000
1	6.699659000	3.086573000	22.479865000
5	6.338981000	4.287690000	22.882081000
1	5.508102000	4.720413000	22.153876000
1	7.326263000	4.897754000	23.122174000
1	5.791717000	3.945864000	24.024587000

lin-2-Li[B₅H₁₂] MeCN E = -138.934274753 Ha			
5	2.486793000	0.882534000	3.329351000
5	0.618063000	0.769163000	2.126277000
5	-0.716856000	0.308309000	3.256636000
5	-0.934946000	1.549581000	2.114455000
5	-1.450388000	1.923928000	3.728127000
1	3.373449000	1.341469000	2.668892000
1	2.384455000	1.417643000	4.414243000
1	1.045307000	0.117608000	1.235003000
1	-1.427943000	-0.619435000	2.995905000
1	-1.717606000	1.312335000	1.258109000
1	-0.765691000	2.518730000	4.528660000
1	-2.623653000	2.053531000	3.901110000
1	1.433205000	1.517205000	2.765731000
1	0.201243000	1.890306000	1.511197000
1	-1.198019000	2.716308000	2.660990000
1	-0.007675000	0.056350000	4.189298000
3	0.617150000	1.458659000	5.197765000
1	2.399737000	-0.306864000	3.352836000

{lin-2-Li[B₅H₁₁]₁ MeCN E = -138.201028772 Ha			
5	1.384722000	0.406152000	3.523078000
5	0.745439000		

5	2.964073000	1.492162000	23.787362000
1	4.332746000	3.448491000	23.006352000
5	5.377929000	2.815552000	22.537451000
1	5.117315000	2.377438000	21.463611000
1	5.421510000	1.837499000	23.399160000
1	6.335025000	3.520441000	22.688798000
1	2.815398000	-0.556677000	25.109756000
5	2.992657000	-0.163699000	23.986996000
1	1.898134000	2.023365000	23.667309000
1	4.121404000	-0.709747000	23.516201000
5	3.272816000	-1.414011000	22.821755000
1	3.466502000	-1.203425000	21.673322000
1	2.164806000	-0.803969000	23.162200000
1	3.259303000	-2.554388000	23.187116000
3	2.932822000	-2.614828000	25.170376000
lin-cyc-Li[B₃H₂] MeCN E = -138.887743093 Ha			
5	4.050797000	2.198802000	22.420588000
1	3.231571000	2.266284000	21.499866000
5	3.383736000	1.408159000	23.721254000
1	5.100929000	1.742113000	22.007419000
5	4.261081000	3.663726000	23.375317000
1	4.039957000	4.794541000	22.970910000
1	5.212155000	3.648899000	24.113956000
1	4.239500000	1.292798000	24.739689000
5	3.764473000	0.077585000	24.782717000
1	2.974921000	0.126089000	23.745194000
1	4.659394000	-0.645092000	24.486482000
1	3.144239000	-0.080564000	25.781829000
3	2.971065000	4.059027000	21.588674000
1	2.312545000	1.842184000	24.322511000
5	2.313363000	3.166494000	24.248777000
1	1.708892000	3.327245000	25.273439000
1	3.413441000	3.709991000	24.531735000
1	1.715938000	3.475476000	23.261395000
{lin-cyc-Li[B₃H₁]}* MeCN E = -138.183998926 Ha			
5	4.006220000	2.315559000	22.646382000
1	5.531848000	2.133161000	21.555373000
5	3.464671000	1.342818000	23.949941000
1	5.185593000	2.149068000	22.744147000
5	4.178446000	4.019298000	23.355588000
1	3.811280000	4.967062000	22.711078000
1	5.203705000	4.136454000	23.938384000
1	4.409334000	0.857537000	24.683747000
5	3.562005000	-0.194201000	24.674816000
1	2.674385000	0.335773000	23.803607000
1	4.113771000	-1.058382000	24.090334000
1	3.070274000	-0.333189000	25.373652000
3	2.796202000	3.899693000	21.297850000
1	2.832365000	2.116697000	24.826898000
5	2.880788000	2.964405000	23.779333000
1	3.295072000	3.986151000	24.425892000
1	1.773144000	3.096143000	23.377290000
1,1-BBB-Li[B₃H₂] MeCN E = -138.875412557 Ha			
5	3.968862000	2.155810000	22.252302000
1	3.522351000	2.480558000	21.205163000
5	3.397736000	1.865778000	23.682015000
1	5.272848000	2.425595000	22.284051000
5	4.812772000	3.151243000	23.316927000
1	5.447234000	2.859726000	24.277213000
1	4.892589000	4.311710000	22.990485000
1	3.809148000	1.549227000	24.808905000
5	3.956159000	0.165933000	24.740006000
1	2.986653000	-0.398694000	24.315688000
1	4.999503000	-0.078162000	24.202920000
1	4.009073000	0.200555000	25.944221000
3	2.936949000	4.767993000	23.154645000
1	2.128712000	1.901482000	23.680219000
5	1.720547000	3.069767000	24.230553000

1	0.816251000	2.589950000	24.848660000
1	2.495869000	3.694786000	24.910675000
1	1.366352000	3.645953000	23.224128000
{1,1-BBB-Li[B₃H₁]}* MeCN E = -138.197340220 Ha			
5	4.180447000	1.454584000	22.946456000
1	3.634829000	1.589127000	21.909305000
5	3.243246000	1.904158000	24.344624000
1	5.207240000	2.308928000	22.942522000
5	4.608248000	2.921989000	23.946168000
1	5.356359000	2.943709000	24.858843000
1	4.419032000	4.018756000	23.427010000
1	3.209971000	1.735646000	25.515327000
5	3.832152000	0.158327000	24.016764000
1	3.055837000	-0.626933000	23.582342000
1	4.797865000	0.340988000	23.044520000
1	4.500643000	-0.121800000	24.955524000
3	1.488522000	5.363912000	23.063871000
1	2.134946000	2.287543000	23.893369000
5	2.917772000	3.510323000	23.697594000
1	2.546335000	4.297775000	24.518439000
1	2.589914000	3.682229000	22.557437000
lin-BB-Li[B₃H₂] MeCN E = -138.846402650 Ha			
5	4.443639000	2.626841000	21.866791000
1	2.362434000	3.244444000	23.172718000
5	2.777414000	2.132444000	23.078402000
1	1.957088000	1.302282000	22.829514000
1	3.547325000	1.740630000	22.084026000
5	5.498259000	3.233389000	22.787704000
1	4.416578000	2.681244000	20.675086000
1	3.389271000	2.037116000	24.196880000
5	3.783851000	0.783889000	24.507384000
1	3.926942000	0.032725000	23.576475000
1	2.979659000	0.416160000	25.310481000
1	4.833529000	1.161738000	24.981928000
3	5.762451000	0.769441000	23.116016000
1	6.512891000	3.968079000	22.425236000
5	6.674474000	3.986079000	23.737843000
1	6.581689000	5.119751000	24.085786000
1	7.621056000	3.348534000	24.072373000
1	5.540087000	3.393305000	24.800548000
{lin-BB-Li[B₃H₁]}* MeCN E = -138.157999783 Ha			
5	4.887562000	2.275933000	21.355494000
1	2.658773000	3.582114000	23.780576000
5	3.495381000	2.744466000	23.678254000
1	2.851128000	1.653351000	23.243944000
1	5.082699000	1.097819000	21.196697000
5	4.955785000	3.004658000	22.834317000
1	4.480714000	2.813064000	20.374206000
1	3.746141000	2.276060000	24.898607000
5	3.201377000	1.193898000	24.409708000
1	4.053213000	0.358379000	24.298577000
1	2.226065000	0.928564000	25.027283000
3	5.335534000	-0.242650000	22.720516000
1	5.278758000	4.287568000	22.807002000
5	6.231612000	3.882203000	23.613350000
1	6.039036000	4.299544000	24.709473000
1	7.274682000	4.066726000	23.076081000
1	5.976649000	2.594447000	23.579179000
B₂H₂ MeCN E = -50.7115834790 Ha			
5	0.761432000	-0.000289000	-0.000015000
5	-0.761432000	0.000212000	-0.000046000
1	-1.929791000	-0.000303000	0.000182000
1	1.929793000	0.000685000	0.000121000
B₂H⁺ MeCN E = -49.7720084214 Ha			
5	0.000000000	0.000000000	0.581202000
5	0.000000000	0.000000000	-0.930111000
1	0.000000000	0.000000000	1.744545000

B₃H₅_conf0_MeCN E = -77.4600558437 Ha			
5	4.567786000	1.664778000	22.321974000
5	3.737043000	1.788421000	23.656462000
1	3.510391000	0.861926000	22.878280000
1	5.209998000	3.788940000	23.935268000
5	4.876162000	2.857331000	23.305669000
1	4.794257000	1.093060000	21.318308000
1	5.517586000	2.742568000	22.260705000
1	3.044750000	1.758395000	24.602971000
B₃H₄⁺_conf0_MeCN E = -76.6147264255 Ha			
5	-0.125084000	5.579068000	5.991059000
1	-0.575505000	8.108425000	6.606915000
5	-0.271925000	7.010062000	6.387032000
1	-1.202905000	6.134940000	5.723182000
5	1.118826000	6.044576000	6.671345000
1	2.155013000	6.208630000	7.167485000
1	0.793231000	4.754790000	6.125709000
B₃H₅_conf1_MeCN E = -77.4281949133 Ha			
5	4.520245000	2.072672000	22.336458000
1	2.268091000	2.688081000	23.147401000
5	3.226484000	1.998639000	23.321561000
1	6.780492000	2.690023000	23.126939000
5	5.817963000	3.039174000	22.513779000
1	4.516476000	1.343019000	21.381310000
1	5.857462000	4.129757000	22.030682000
1	3.185927000	1.248967000	24.249340000
B₃H₄⁺_conf1_MeCN E = -76.5958090969 Ha			
5	4.413546000	2.046669000	22.252810000
1	2.143509000	2.501970000	23.074293000
5	3.181653000	1.975562000	23.318967000
5	5.521736000	3.263542000	22.283705000
1	4.533604000	1.220270000	21.406401000
1	6.303463000	4.133568000	22.303333000
1	3.295137000	1.378730000	24.341022000
arachno-B₃H₅_conf0_MeCN E = -104.116408480 Ha			
5	1.148677000	5.741231000	5.237547000
5	0.385320000	5.238908000	6.682893000
1	0.327549000	4.431174000	7.540149000
1	-0.888305000	5.729659000	6.383126000
1	1.989959000	5.230671000	4.584515000
1	0.049787000	6.070304000	4.501827000
5	-0.450990000	5.152798000	5.304641000
1	-1.217243000	4.489570000	4.709611000
1	1.502905000	7.018759000	5.456947000
5	1.428604000	6.637734000	6.727272000
1	0.739025000	7.519448000	7.146764000
1	2.554607000	6.560157000	7.111777000
arachno-B₃H₄⁺_conf0_MeCN E = -103.305001843 Ha			
5	1.169552000	5.590198000	5.121516000
5	0.483707000	5.090303000	6.656680000
1	0.480318000	4.198173000	4.721801000
1	-0.693424000	5.695627000	6.581545000
1	1.959418000	5.109275000	4.398352000
1	0.137205000	6.099822000	4.490063000
5	-0.464527000	5.210279000	5.338430000
1	-1.420033000	4.824334000	4.787110000
1	1.768040000	6.812863000	5.438223000
5	1.476565000	6.439729000	6.638574000
1	1.934047000	7.230357000	7.368031000
disph-B₃H₅_MeCN E = -104.104903539 Ha			
5	3.783974000	1.304255000	22.454652000
1	1.846133000	2.756116000	23.588544000
5	2.992496000	2.588647000	23.433193000
1	2.736285000	0.940149000	22.022475000
5	4.496071000	2.775355000	23.204443000

1	4.714941000	1.188367000	21.721617000
1	5.562472000	3.218233000	23.022647000
1	3.610397000	3.708684000	23.276376000
5	4.050539000	1.418491000	24.297091000
1	5.151839000	1.373663000	24.747146000

1	1.585976000	1.469462000	25.272394000
sq-BaH₂ MeCN E = -104.079044407 Ha			
5	5.259178000	1.707259000	23.336362000
5	2.816143000	1.675312000	23.266266000
1	4.881444000	2.823597000	23.973297000
5	4.025245000	2.859036000	22.943275000
1	4.025215000	3.998170000	22.593502000
1	4.939857000	2.269067000	22.163149000
1	3.135688000	1.113114000	24.439286000
5	4.049544000	0.523500000	23.658549000
1	3.193270000	0.559529000	22.628757000
1	1.625110000	1.650941000	23.239360000
1	4.050272000	-0.616203000	24.006477000
1	6.450417000	1.732346000	23.364239000

sq-BaH₂ MeCN E = -103.307400134 Ha			
5	5.091885000	1.845834000	23.286619000
5	3.348764000	1.611369000	23.302251000
1	4.973028000	3.017908000	23.908523000
5	4.073186000	3.034563000	22.891275000
1	3.866887000	4.134498000	22.548759000
1	5.029951000	2.470564000	22.111881000
1	3.063862000	1.088274000	24.460245000
5	3.913678000	0.295167000	23.725089000
1	3.127013000	0.525072000	22.619926000
1	4.166140000	-0.786099000	24.064879000
1	6.171880000	1.407578000	23.453712000

lin-BBB-BaH₂ MeCN E = -104.071572706 Ha			
5	4.775836000	1.655097000	22.424577000
5	3.824390000	1.859638000	23.868843000
1	3.586045000	1.122159000	22.816205000
1	5.708838000	3.741079000	23.747271000
5	5.008383000	2.852383000	23.424748000
1	5.020464000	0.960630000	21.499210000
1	4.701823000	2.915305000	22.102195000
1	4.047752000	1.062912000	24.914661000
5	2.771990000	1.255862000	25.103516000
1	2.197697000	0.233338000	24.924414000
1	2.513431000	2.107795000	24.165769000
1	2.674912000	1.853171000	26.124528000

lin-BBB-BaH₂ MeCN E = -103.301265907 Ha			
5	4.858358000	1.630184000	22.403854000
5	4.014644000	1.208454000	23.708286000
1	3.748263000	0.835950000	22.493992000
1	5.002333000	3.665577000	24.131496000
5	4.580064000	2.692439000	23.638117000
1	5.520189000	1.268962000	21.512441000
1	4.515981000	2.889213000	22.297590000
1	3.529262000	0.580990000	24.619551000
5	3.183127000	2.113236000	24.850967000
1	2.025765000	2.189502000	24.627886000
1	3.655876000	2.334417000	25.907343000

arachno-BsH₁₀ MeCN E = -130.76422891 Ha			
5	1.748326000	0.872717000	3.248088000
5	0.768665000	0.898009000	1.817996000
5	-0.064235000	0.397827000	3.252437000
5	-0.909816000	1.391359000	2.098940000
5	-1.092891000	1.825462000	3.834162000
1	2.554412000	0.000403000	3.190503000
1	1.936731000	1.771343000	4.003727000
1	0.916164000	0.123392000	0.939468000
1	-0.424993000	-0.722889000	3.380201000
1	-1.738085000	0.945725000	1.386487000
1	-0.561918000	2.763823000	4.348702000
1	-2.158769000	1.501101000	4.244090000
1	1.839301000	1.562904000	2.058550000
1	0.047567000	1.948483000	1.378928000
1	-1.292196000	2.481458000	2.614365000

1	0.047611000	1.020451000	4.321711000
arachno-BsH₁₀ MeCN E = -129.959629281 Ha			
5	1.881251000	0.596483000	3.182269000
5	0.811585000	1.163848000	1.960710000
5	0.008918000	0.552438000	3.404786000
5	-0.826697000	1.781157000	2.348879000
5	-1.106649000	1.607985000	4.013601000
1	2.397756000	-0.368489000	2.742021000
1	2.238224000	1.098730000	4.189286000
1	0.700758000	0.582717000	0.943688000
1	-0.241528000	-0.543215000	3.770006000
1	-1.125937000	2.700400000	3.249635000
1	-1.997740000	1.604921000	4.766020000
1	1.967532000	1.614080000	2.229362000
1	0.243598000	2.686323000	1.891013000
1	-1.675229000	1.716335000	1.543086000
1	0.078107000	1.342131000	4.497507000

lin-1-BsH₁₁ conf0 MeCN E = -130.736549045 Ha			
5	4.511240000	1.375163000	22.708919000
1	5.133590000	0.579824000	22.095984000
5	2.906770000	1.908408000	23.367200000
1	5.240367000	1.857510000	23.703278000
5	4.312356000	2.802966000	23.425811000
1	4.722209000	3.874424000	23.662543000
1	4.569029000	2.514919000	22.075133000
1	2.623646000	1.111261000	24.407989000
5	3.124979000	0.304248000	23.478848000
1	2.298175000	-0.519887000	22.952955000
1	1.942630000	2.141151000	22.725101000
1	3.924547000	-0.434534000	24.159334000
5	3.059895000	-1.375955000	23.680872000
1	3.667059000	-2.032928000	22.915305000
1	2.425126000	-1.783218000	24.584481000

lin-1-BsH₁₀ conf0 MeCN E = -129.962460154 Ha			
5	4.409773000	1.359641000	22.683087000
1	4.940214000	0.598008000	21.951909000
5	2.973317000	1.774063000	23.711117000
1	5.309077000	1.963477000	23.444811000
5	4.246974000	2.799415000	23.386660000
1	4.587031000	3.916270000	23.481032000
1	4.184698000	2.464396000	22.024499000
1	3.040729000	1.001563000	24.805923000
5	3.381407000	0.205083000	23.800168000
1	1.861004000	1.878932000	23.326322000
1	4.397868000	-0.418202000	24.277268000
5	3.552178000	-1.462465000	24.045042000
1	3.207146000	-1.893150000	25.084438000
1	4.021977000	-2.086160000	23.163533000
1	2.545632000	-0.720238000	23.512945000

commo-BsH₁₁ conf0 MeCN E = -130.733269276 Ha			
5	1.971552000	0.606675000	5.982603000
1	-0.261862000	6.635236000	5.358669000
5	0.493606000	0.962851000	6.222400000
1	-0.049605000	6.587806000	7.345863000
5	0.964835000	5.739882000	7.410772000
1	0.712348000	8.122125000	6.377816000
1	0.482433000	4.653536000	7.393389000
5	2.587009000	7.041448000	4.671245000
1	1.786457000	7.146824000	3.797611000
1	3.039131000	8.034498000	5.154463000
1	1.619161000	6.058670000	8.355613000
1	3.586462000	6.415767000	4.115045000
5	3.381188000	5.508285000	5.054411000
1	2.417524000	5.099632000	6.545829000
1	4.377719000	5.478301000	5.701601000
1	3.027584000	4.511002000	4.503390000

commo-BsH₁₀ conf0 MeCN E = -129.938379161 Ha			
5	1.969104000	6.268054000	5.935558000
1	-0.541157000	5.935815000	5.606441000
5	0.197580000	6.690057000	6.141412000
1	-0.006811000	6.762387000	7.441306000
5	1.076658000	6.045821000	7.484213000
1	0.295474000	7.812617000	5.754723000
1	0.850448000	4.915494000	7.752600000
5	2.778347000	7.048989000	4.730868000
1	2.780465000	7.991326000	4.044370000
1	2.793583000	7.323989000	6.018676000
1	1.878552000	6.656449000	8.127801000
1	3.723499000	6.167034000	4.391030000
5	2.694109000	5.401256000	4.726939000
1	2.641304000	5.136240000	6.045326000
1	2.626686000	4.428776000	4.088200000

commo-BsH₁₁ conf1 MeCN E = -130.735128900 Ha			
5	4.516699000	2.167930000	22.809162000
1	3.819367000	3.399659000	24.596970000
5	3.356021000	2.921695000	23.968195000
1	2.653932000	3.628326000	23.309227000
1	4.268018000	2.192011000	21.643829000
1	7.169206000	1.357145000	23.311818000
5	6.310601000	2.153011000	23.257344000
1	2.517941000	1.995429000	24.396188000
5	3.402107000	1.174976000	23.870961000
1	5.114892000	1.101950000	23.083106000
1	2.740439000	0.506706000	23.136015000
1	3.923065000	0.622354000	24.795749000
1	6.663239000	3.199638000	22.565136000
5	5.549145000	3.495861000	23.314500000
1	5.432178000	4.656711000	23.382261000
1	6.179496000	2.888819000	24.349614000

commo-BsH₁₀ conf1 MeCN E = -129.955491048 Ha			
5	4.587448000	2.084682000	22.946866000
1	3.666280000	2.191819000	25.178095000
5	3.443569000	2.932310000	24.097409000
1	3.260359000	4.070005000	24.281324000
1	4.302769000	1.753310000	21.843162000
1	7.322059000	1.731119000	23.698061000
5	6.375101000	2.338169000	23.366241000
1	2.356636000	2.211735000	23.850150000
5	3.393425000	1.420139000	24.118861000
1	5.390470000	1.239060000	23.444204000
1	3.143515000	0.300141000	24.320810000
1	6.614222000	3.044454000	22.290525000
5	5.511987000	3.556057000	22.909524000
1	5.321941000	4.662761000	22.591591000
1	6.186124000	3.428000000	24.086238000

commo-BsH₁₁ conf2 MeCN E = -130.734955123 Ha			
1	0.927313000	5.857283000	4.442042000
5	1.598339000	6.282328000	5.323490000
1	-0.693101000	5.609869000	6.100511000
5	0.006601000	6.570004000	6.160163000
1	0.213411000	6.815762000	7.444587000
5	1.437128000	6.500120000	7.119798000
1	-0.389563000	7.593022000	5.692183000
1	1.711027000	5.457874000	7.636223000
5	3.168628000	6.782336000	5.161195000
1	2.117139000	7.428943000	4.761035000
1	3.923982000	7.431903000	7.810740000
1	2.071751000	7.457807000	7.438085000
1	3.710932000	6.117848000	4.173888000
5	3.121892000	5.132765000	6.176966000
1	3.941641000	4.730697000	5.690124000
1	2.630482000	4.387484000	4.159368000

commo-BsH₁₀ conf2 MeCN E = -129.946959015 Ha			
1	0.928300000	5.649624000	

lin-BBB-B₅H₁₀⁺_conf0_MeCN E = -129.955628485 Ha

5	4.278463000	2.933092000	22.873214000
1	4.008998000	2.241040000	25.506255000
5	3.857124000	1.982262000	24.378696000
1	2.626907000	1.623069000	24.037759000
1	4.991716000	2.356107000	22.001220000
1	5.378964000	4.480441000	24.799865000
5	5.425495000	3.803767000	23.850124000
1	3.538263000	3.692471000	22.339652000
1	4.296824000	0.790270000	23.988385000
5	3.489333000	1.326500000	23.065874000
1	3.087478000	0.625816000	22.226207000
1	6.442618000	2.898150000	23.864160000
5	6.101385000	3.139305000	22.611882000
1	6.938709000	2.849310000	21.843970000
1	6.078165000	4.429254000	22.829338000

bis-BH-B₅H₁₁_MeCN E = -130.720923528 Ha

5	4.315194000	2.440212000	23.862617000
1	4.604961000	2.929469000	24.913445000
5	2.954648000	1.478426000	23.790696000
1	4.326701000	3.417153000	22.959007000
5	5.381745000	2.776113000	22.529641000
1	5.140730000	2.307314000	21.463603000
1	5.414255000	1.822846000	23.416004000
1	6.334619000	3.471021000	22.675063000
1	2.814975000	-0.581369000	25.144366000
5	2.987815000	-0.170749000	24.035808000
1	1.889736000	2.009494000	23.642794000
1	4.113826000	-0.740100000	23.592968000
5	3.286661000	-1.362263000	22.804167000
1	3.471080000	-1.003990000	21.685402000
1	2.166698000	-0.844352000	23.234851000
1	3.297112000	-2.520770000	23.069663000

bis-BH-B₅H₁₀⁺_MeCN E = -129.941346488 Ha

5	4.409773000	1.359641000	22.683087000
1	4.940214000	0.598008000	21.951909000
5	2.973317000	1.774063000	23.711117000
1	5.309077000	1.963477000	23.444811000
5	4.246974000	2.799415000	23.386660000
1	4.587031000	3.916270000	23.481032000
1	4.184698000	2.464396000	22.024499000
1	3.040729000	1.001563000	24.805923000
5	3.381407000	0.205083000	23.800168000
1	1.861004000	1.878932000	23.326322000
1	4.397868000	-0.418202000	24.277268000
5	3.552178000	-1.462465000	24.045042000
1	3.207146000	-1.893150000	25.084438000
1	4.021977000	-2.086160000	23.163533000
1	2.545632000	-0.720238000	23.512945000

i-bis-B₄H₈(BH₃)_MeCN E = -130.719355925 Ha

5	4.913023000	2.550384000	21.106509000
1	2.412002000	3.161126000	23.213392000
5	3.413851000	2.583507000	23.497364000
1	3.143649000	1.287703000	23.449231000
1	5.219937000	1.467600000	20.706292000
5	4.888761000	2.918993000	22.720474000
1	4.518305000	3.316544000	20.279460000
1	3.547067000	2.657855000	24.195490000
5	3.293120000	1.378662000	24.748953000
1	4.272501000	0.781321000	25.062517000
1	2.251894000	1.149934000	25.272316000
5	5.234931000	4.179083000	22.972941000
5	6.189104000	3.598725000	23.657011000
1	6.016183000	3.807165000	24.816713000
1	7.233943000	3.864160000	23.155242000
1	5.891301000	2.356032000	23.404782000

i-bis-B₄H₈(BH₂)⁺_MeCN E = -129.944862992 Ha

5	4.305787000	2.745661000	21.647043000
1	2.879704000	2.396614000	21.736735000
5	3.244398000	2.394828000	22.939158000
1	3.029636000	1.316803000	23.636101000
1	4.714385000	1.821227000	21.030828000
5	4.823343000	2.731420000	23.400340000
1	4.234109000	3.834256000	21.187621000
1	2.602679000	2.337570000	23.774328000
5	3.497641000	2.336136000	24.465134000
1	3.224901000	2.187280000	25.587847000
1	5.343657000	3.876465000	23.677208000
5	6.458834000	3.104690000	23.683285000
1	6.870110000	3.118113000	24.789415000
1	7.124031000	3.335960000	22.736503000
1	5.813857000	1.919390000	23.528681000

lin-B₅H₁₁_conf1_MeCN E = -130.704799304 Ha

5	4.426365000	1.423737000	22.584083000
1	5.030148000	0.804453000	21.774821000
5	2.863348000	1.886129000	23.311570000
1	5.158822000	1.614862000	23.677385000
5	4.307118000	2.670650000	23.600517000
1	4.797269000	3.621797000	24.087027000
1	4.621800000	2.697844000	22.261583000
1	2.497710000	0.939479000	24.124817000
5	2.993111000	0.229594000	23.073654000
1	2.220285000	-0.353105000	22.400547000
1	1.953611000	2.354312000	22.711619000
1	3.960586000	-0.373678000	23.591407000
5	3.531179000	-1.490130000	24.371643000
1	4.417693000	-1.295826000	25.155551000
1	3.679235000	-2.379560000	23.586857000
1	2.421031000	-1.323032000	24.786222000

lin-B₅H₁₀⁺_conf1_MeCN E = -129.941346488 Ha

5	4.409773000	1.359641000	22.683087000
1	4.940214000	0.598008000	21.951909000
5	2.973317000	1.774063000	23.711117000
1	5.309077000	1.963477000	23.444811000
5	4.246974000	2.799415000	23.386660000
1	4.587031000	3.916270000	23.481032000
1	4.184698000	2.464396000	22.024499000
1	3.040729000	1.001563000	24.805923000
5	3.381407000	0.205083000	23.800168000
1	1.861004000	1.878932000	23.326322000
1	4.397868000	-0.418202000	24.277268000
5	3.552178000	-1.462465000	24.045042000
1	3.207146000	-1.893150000	25.084438000
1	4.021977000	-2.086160000	23.163533000
1	2.545632000	-0.720238000	23.512945000

bis-BH₂-B₅H₁₁_MeCN E = -130.698438386 Ha

5	4.516775000	2.426707000	22.420829000
1	2.846733000	3.143808000	24.248318000
5	3.377711000	2.233244000	23.676390000
1	2.376341000	1.397576000	23.317485000
1	4.903383000	1.360853000	21.965749000
1	6.632214000	2.859581000	24.061927000
5	5.809811000	3.250482000	23.021332000
1	4.036971000	3.122558000	21.537558000
1	3.826328000	1.407908000	24.649848000
5	2.823131000	0.678402000	24.291654000
1	2.018882000	0.627737000	25.169466000
1	3.252719000	-0.334451000	23.830072000
1	6.965331000	3.662339000	22.370741000
5	6.990618000	4.017464000	23.610271000
1	7.884865000	4.605469000	24.066222000
1	5.786760000	4.497841000	23.606062000

bis-BH₂-B₅H₁₀⁺_MeCN E = -129.939066112 Ha

5	5.333395000	2.220981000	21.867680000
1	3.535831000	2.892043000	25.581228000
5	3.729267000	2.321515000	24.560517000
1	2.600737000	2.189560000	23.919338000
1	4.559109000	1.333035000	21.908192000
1	6.137376000	3.107676000	23.959378000
5	4.893857000	2.913081000	23.511879000
1	6.020373000	2.337571000	20.916128000
1	3.972557000	1.064418000	24.810874000
5	2.786450000	0.908188000	24.227689000
1	1.988369000	0.571817000	25.033457000
1	2.945590000	3.062380000	23.219834000
1	6.827229000	4.338914000	22.351060000
5	5.985972000	3.648671000	22.760046000
1	4.847596000	4.198947000	23.150403000

lin-BB-B₅H₁₁_MeCN E = -130.681068004 Ha

5	4.088893000	2.769937000	22.036531000
1	2.971177000	3.073278000	22.690209000
5	2.958812000	1.775490000	22.897913000
1	1.961583000	1.325586000	22.463715000
1	3.998081000	1.445130000	22.204124000
5	5.458147000	3.358220000	22.749333000
1	3.852007000	2.954534000	20.888480000
1	3.095688000	1.851998000	24.149899000
5	3.643133000	0.657581000	24.542143000
1	3.541308000	-0.181440000	23.689037000
1	2.887943000	0.520119000	25.460926000
1	4.759962000	1.010277000	24.793207000
1	5.903575000	4.587993000	22.479770000
5	6.658786000	3.934436000	23.367022000
1	7.540341000	4.491184000	23.894283000
1	5.532797000	3.699035000	24.043119000

lin-BB-B₅H₁₀⁺_MeCN E = -129.907084287 Ha

5	4.197771000	2.847528000	22.265438000
1	3.227858000	2.891253000	23.278198000
5	3.416138000	1.648563000	23.185904000
1	2.359935000	1.031791000	22.827644000
1	4.364948000	1.465516000	22.373358000
5	5.580051000	3.610689000	22.694103000
1	3.609027000	3.025008000	21.257282000
1	3.731815000	1.168941000	24.324692000
5	2.601819000	0.441105000	24.042789000
1	2.934987000	-0.668320000	23.841582000
1	1.758518000	0.791298000	24.783447000
1	5.777748000	4.882563000	22.401707000
5	6.832686000	4.302622000	23.008141000
1	7.743299000	4.954011000	23.336137000
1	5.955671000	3.870512000	23.935029000

1,2-BBB-B₅H₁₁_conf1_MeCN E = -130.673977162 Ha

5	4.600558000	2.541792000	21.526241000
5	3.731774000	2.271953000	22.949359000
1	2.553807000	2.360452000	22.888373000
1	4.186439000	1.386302000	22.003541000
5	5.402920000	3.260999000	22.631139000
1	4.062628000	2.807727000	20.511739000
1	4.275610000	2.069058000	24.042233000
5	3.842346000	0.809637000	24.590120000
1	3.423597000	0.051953000	23.765240000
1	3.054231000	1.208286000	25.395331000
1	4.961188000	0.604085000	24.973271000
1	5.603577000	4.539378000	22.698447000
5	6.240667000	4.131486000	23.802723000
1	5.631981000	4.401873000	24.780359000
1	7.374285000	4.434931000	23.656809000
1	6.214461000	2.812928000	23.526394000

1	6.003830000	-1.701612000	-1.340271000
[B₅H₄]⁻_ap_MeCN E = -126.602717680 Ha			
5	4.603196000	-1.078245000	0.873663000
5	4.913211000	-1.345604000	-0.623079000
5	3.030310000	-0.426336000	0.477284000
5	3.388327000	-1.595866000	-0.768788000
5	4.096758000	0.165393000	-0.494563000
1	2.521145000	-2.287074000	-1.191950000
1	4.884550000	-1.277328000	2.009324000
1	4.446747000	1.155819000	-1.065270000
1	2.090842000	-0.501163000	1.201187000
[B₅H₄]⁻_eq_MeCN E = -126.639100797 Ha			
5	4.403736000	-1.024875000	0.886930000
5	5.090097000	-1.154698000	-0.828498000
5	2.873264000	-0.505940000	0.624844000
5	3.271223000	-1.492675000	-0.614826000
5	4.124206000	-0.080998000	-0.445793000
1	2.911954000	-2.452282000	-1.209823000
1	5.083679000	-1.548280000	1.703915000
1	1.955617000	0.036428000	1.151292000
1	5.946343000	-1.840025000	-1.258657000
[B₅H₄]²⁻_MeCN E = -152.929889855 Ha			
5	1.218442000	-0.002599000	0.112491000
1	2.418507000	-0.121020000	0.115197000
5	0.012376000	1.222906000	0.151577000
5	-0.000493000	-0.034082000	1.325378000
5	0.005307000	0.049161000	-1.105522000
5	-1.213638000	0.017698000	0.107396000
5	-0.007594000	-1.207816000	0.068309000
1	-2.413704000	0.027354000	0.105059000
1	0.007879000	0.087931000	-2.304939000
1	-0.016678000	-2.407221000	0.029693000
1	-0.003074000	-0.072835000	2.524789000
1	0.021555000	2.422294000	0.190299000
[B₅H₄]⁻_MeCN E = -152.145398235 Ha			
5	1.016915000	-0.000630000	0.112002000
5	0.017165000	1.284429000	0.152647000
5	0.003968000	-0.035126000	1.386923000
5	0.009830000	0.050226000	-1.167034000
5	-1.116609000	0.016540000	0.107696000
5	-0.003346000	-1.269451000	0.067243000
1	-2.307248000	0.026377000	0.105247000
1	0.003086000	0.090017000	-2.350141000
1	-0.022368000	-2.452427000	0.027590000
1	-0.008249000	-0.074723000	2.569993000
1	0.017234000	2.467559000	0.192363000
[B₅H₄]²⁻_MeCN E = -178.390435612 Ha			
5	8.299703000	19.095461000	4.107398000
1	9.121194000	18.975959000	4.972105000
5	6.937472000	20.019415000	4.193295000
1	6.598823000	20.685761000	5.130442000
5	6.126735000	19.864980000	2.767361000
1	5.093392000	20.399260000	2.478158000
5	6.987458000	18.844278000	1.801502000
1	6.689352000	18.507597000	0.689885000
5	8.331002000	18.368417000	2.629262000
1	9.180338000	17.624812000	2.225999000
5	7.912105000	20.126092000	2.675713000
1	8.520031000	21.064488000	2.227156000
5	6.760676000	18.351084000	3.523774000
1	6.152729000	17.412691000	3.972327000
[B₅H₄]⁻_ap_MeCN E = -177.631934001 Ha			
5	8.322546000	19.080816000	4.144021000
1	9.142969000	18.973018000	4.990842000
5	6.918451000	20.033521000	4.231690000
1	6.590045000	20.704266000	5.150494000

5	6.082861000	19.873467000	2.761535000
1	5.069119000	20.413232000	2.473388000
5	6.970417000	18.821836000	1.765255000
1	6.683480000	18.500681000	0.662244000
5	8.354485000	18.331645000	2.619760000
1	9.201336000	17.608922000	2.216720000
5	7.862356000	20.049562000	2.712428000
1	8.462599000	20.974381000	2.270652000
5	6.897615000	18.562256000	3.423021000
[B₇H₆]⁻_eq_MeCN E = -177.613739297 Ha			
5	8.375116000	19.040521000	4.095070000
1	9.102492000	19.016252000	5.030577000
5	6.979948000	19.988931000	4.186209000
1	6.711086000	20.625963000	5.155674000
5	6.158161000	19.830943000	2.739577000
1	5.135267000	20.323107000	2.379377000
5	7.043900000	18.784500000	1.751994000
1	6.234488000	18.540981000	0.671012000
5	8.240784000	18.447818000	2.672194000
5	7.878646000	20.2107488000	2.686010000
1	8.497649000	21.194787000	2.234929000
5	6.684116000	18.366153000	3.565833000
1	6.100059000	17.423348000	3.999920000
[B₇H₆]²⁻_MeCN E = -203.842628331 Ha			
5	1.597360000	4.449706000	2.296386000
5	1.631042000	4.878782000	3.951855000
1	1.378988000	3.302312000	2.010134000
1	1.446677000	4.086220000	4.829820000
5	0.598767000	5.909642000	2.898473000
5	3.038219000	5.427308000	2.974483000
5	1.084087000	5.827740000	1.260341000
5	2.657989000	5.516946000	1.309423000
5	1.941282000	6.453529000	3.965255000
5	2.079122000	6.890311000	2.317387000
1	-0.557478000	6.135413000	3.139977000
1	4.176708000	5.198978000	3.287506000
1	0.321811000	5.986434000	0.351059000
1	3.475997000	5.362149000	0.449523000
1	2.069769000	7.241701000	4.856785000
1	2.314295000	8.038985000	2.050228000
[B₈H₇]⁻_ap_MeCN E = -203.058784578 Ha			
5	1.609903000	4.370680000	2.365385000
5	1.649458000	4.858379000	3.966220000
1	1.381450000	3.261450000	1.998514000
1	1.442636000	4.140486000	4.892225000
5	0.687459000	5.892126000	2.875806000
5	3.058686000	5.422737000	3.012843000
5	1.082947000	5.829709000	1.096170000
5	2.507071000	5.544763000	1.458967000
5	1.966188000	6.464702000	3.979788000
5	2.120760000	6.956909000	2.387329000
1	-0.483377000	6.122828000	2.916501000
1	4.213064000	5.193683000	3.207946000
1	0.165037000	6.017701000	0.383766000
1	2.045017000	7.192352000	4.917900000
1	2.332341000	8.075571000	2.039751000
[B₈H₇]⁻_eq_MeCN E = -203.084110828 Ha			
5	1.490735000	4.449704000	2.281846000
5	1.647607000	4.855998000	3.972984000
1	1.258101000	3.308340000	2.047781000
1	1.502288000	4.002090000	4.782638000
5	0.610045000	5.907160000	2.939112000
5	2.851028000	5.464489000	2.938066000
5	1.151704000	5.814365000	1.278575000
5	2.798387000	5.488286000	1.366614000
5	1.965745000	6.467619000	3.986878000
5	1.980797000	6.930900000	2.303030000
1	-0.531568000	6.130162000	3.217698000

1	0.546079000	5.942405000	0.259928000
1	3.453965000	5.367770000	0.389537000
1	2.153127000	7.299163000	4.811133000
1	2.199885000	8.078714000	2.088012000
[B₉H₈]²⁻_MeCN E = -229.322982551 Ha			
5	1.639800000	1.663838000	6.855571000
5	0.677705000	0.726092000	7.902333000
5	1.621089000	0.710011000	5.952193000
1	1.657010000	1.691324000	5.662766000
1	-0.025241000	-0.133626000	7.451350000
1	1.628210000	-0.162024000	10.413846000
5	2.612736000	0.770658000	7.931217000
5	2.570870000	2.551735000	7.971659000
5	0.636143000	2.507428000	7.942925000
5	0.183902000	1.574584000	9.293950000
5	3.025538000	1.639515000	9.339532000
1	3.366439000	-0.056271000	7.501301000
5	1.579851000	2.490593000	9.632704000
1	3.285841000	3.430688000	7.580768000
1	-0.105514000	3.353566000	7.529847000
1	-0.855717000	1.536916000	9.878131000
1	4.048856000	1.649251000	9.949987000
1	1.548359000	3.324247000	10.492726000
[B₉H₈]⁻_ap_MeCN E = -228.532455594 Ha			
5	1.619421000	1.593781000	6.796682000
5	0.715156000	0.699108000	7.941277000
5	1.606772000	0.683804000	9.539260000
1	1.875539000	1.628158000	5.637993000
1	-0.020002000	-0.229778000	7.824671000
1	1.312689000	-0.252740000	10.212299000
5	2.571762000	0.764617000	7.953739000
5	2.290429000	2.621225000	8.128462000
5	0.414755000	2.437818000	7.531711000
5	0.599683000	2.057730000	9.066377000
5	3.063359000	1.568978000	9.383644000
1	3.370688000	0.001430000	7.500467000
5	1.812027000	2.413192000	10.035566000
1	2.851304000	3.627754000	7.824842000
1	-0.272895000	3.205347000	6.948588000
1	4.184543000	1.588614000	9.773347000
1	1.951515000	3.167353000	10.937767000
[B₉H₈]⁻_eq_MeCN E = -228.540583622 Ha			
5	1.638936000	1.700539000	6.859800000
5	0.666739000	0.744563000	7.915669000
5	1.622238000	0.663634000	9.586872000
1	1.656114000	1.719606000	5.672039000
1	-0.046801000	-0.117550000	7.504702000
1	1.630201000	-0.207507000	10.387867000
5	2.622164000	0.789268000	7.944611000
5	2.637639000	2.556297000	7.945060000
5	0.570453000	2.509067000	7.914344000
5	0.153089000	1.594297000	9.313672000
5	3.054879000	1.660400000	9.566620000
1	3.385994000	-0.039234000	7.555496000
5	1.586111000	2.348115000	9.430561000
1	3.332359000	3.441163000	7.566375000
1	-0.152487000	3.361330000	7.514307000
1	-0.847723000	1.554650000	9.943369000
1	4.037614000	1.665641000	10.015474000
[B₁₀H₉]²⁻_MeCN E = -254.829971350 Ha			
5	0.329222000	5.335743000	5.514006000
5	3.073272000	4.588887000	6.136002000
5	1.771017000	5.826677000	6.257885000
5	2.521595000	3.594064000	4.715556000
5	3.112644000	6.071636000	5.081973000
5	0.990819000	4.419620000	4.259830000
5	1.408609000	6.171349000	4.507986000
5	3.868991000	4.620819000	4.639190000

5	2.560979000	5.076738000	3.661570000
5	1.353315000	4.074570000	5.998720000
1	3.674521000	4.296405000	7.128620000
1	0.270992000	3.878638000	3.461064000
1	3.748200000	7.08397	

1 0.454316000 19.037828000 14.243253000
1 -1.085124000 16.908684000 14.695758000
1 2.249709000 15.145096000 17.756890000
1 1.882571000 19.959212000 17.073880000
1 -0.906295000 16.106043000 17.893791000
1 1.326409000 17.743912000 18.969341000
1 -0.894797000 18.915396000 16.931351000

[B₁₁H₁₀]_{-ap}_MeCN E = -279.485017945 Ha

5 1.655710000 16.760814000 15.478803000
5 2.559010000 18.193434000 15.319099000
5 0.603545000 15.490972000 15.894823000
5 2.755026000 17.449120000 16.799167000
5 0.918886000 18.418988000 15.113945000
5 -0.190361000 16.866041000 15.440655000
5 1.645806000 15.916380000 17.126005000
5 1.679031000 18.867336000 16.666004000
5 -0.046345000 16.483121000 17.173993000
5 1.268672000 17.533556000 17.791558000
5 0.017497000 18.194422000 16.643162000
1 3.417830000 18.518937000 14.571065000
1 0.442001000 14.406392000 15.446764000
1 3.810483000 17.260590000 17.303373000
1 0.448632000 19.036368000 14.218651000
1 -1.091941000 16.907454000 14.672296000
1 2.269730000 15.131319000 17.757164000
1 1.882097000 19.965017000 17.076643000
1 -0.910690000 16.104710000 17.898080000
1 1.370172000 17.711213000 18.963855000
1 -0.903269000 18.910634000 16.878410000

[B₁₁H₁₀]_{-eq1}_MeCN E = -279.500480098 Ha

5 1.436051000 16.497627000 14.931353000
5 2.426601000 17.602775000 15.760373000
5 0.531818000 15.470829000 15.908418000
5 2.900014000 17.617459000 17.235683000
5 0.960108000 18.231308000 15.136828000
5 -0.242569000 16.961574000 15.407610000
5 1.865110000 16.133885000 16.708056000
5 1.641456000 18.870164000 16.660996000
5 -0.004141000 16.493216000 17.120906000
5 1.246478000 17.602619000 17.800076000
5 0.012301000 18.199492000 16.670198000
1 1.958296000 16.042518000 13.962473000
1 0.287995000 14.331380000 15.700557000
1 3.788023000 17.662521000 18.006737000
1 0.910047000 18.986292000 14.222130000
1 -1.245434000 16.934377000 14.768724000
1 2.562139000 15.262817000 17.194122000
1 1.911185000 20.015533000 16.798886000
1 -0.784768000 16.107219000 17.932497000
1 1.229940000 17.639692000 18.988814000
1 -0.888346000 18.917507000 16.965127000

[B₁₁H₁₀]_{-eq2}_MeCN E = -279.500500166 Ha

5 1.850940000 16.647757000 15.269050000
5 2.574297000 18.212891000 15.340682000
5 0.491614000 15.488209000 15.803126000
5 2.708142000 17.431268000 16.814914000
5 0.910028000 18.331063000 15.134316000
5 0.024195000 16.946468000 15.568218000
5 1.614836000 16.012224000 17.035285000
5 1.662338000 18.880168000 16.680872000
5 -0.041443000 16.529282000 17.258097000
5 1.266319000 17.565515000 17.823757000
5 0.017321000 18.228061000 16.704856000
1 2.318102000 16.017621000 14.374589000
1 3.408027000 18.666543000 14.633608000
1 0.384114000 14.344013000 15.549104000
1 3.773155000 17.290781000 17.327759000
1 0.497622000 18.854968000 14.147358000

1 2.175198000 15.068392000 17.493436000
1 1.879191000 19.983831000 17.067189000
1 -0.926807000 16.115883000 17.927992000
1 1.355162000 17.769523000 18.991764000
1 -0.938866000 18.892800000 16.934624000

[B₁₂H₁₂]²⁻_MeCN E = -305.838190013 Ha

5 -0.789798000 -0.933910000 1.182040000
5 0.379520000 0.325520000 1.614424000
1 -1.362355000 -1.570183000 2.015677000
1 0.633994000 0.579427000 2.753683000
5 0.933935000 -1.173015000 0.848661000
1 1.582212000 -1.980812000 1.444305000
5 -0.276057000 -1.654587000 -0.353052000
1 -0.484477000 -2.803171000 -0.607126000
5 -1.173182000 0.770430000 0.885956000
1 -2.019191000 1.341098000 1.507393000
5 -1.578648000 -0.453458000 -0.329925000
1 -2.711372000 -0.748310000 -0.569012000
5 1.210375000 -0.840392000 -0.869540000
1 2.056371000 -1.4111047000 -1.491011000
5 1.615839000 0.383500000 0.346337000
1 2.748553000 0.678390000 0.585432000
5 -0.896756000 1.103061000 -0.832255000
1 -1.545038000 1.910863000 -1.427887000
5 0.313243000 1.584622000 0.369450000
1 0.521678000 2.733210000 0.623493000
5 0.826984000 0.863950000 -1.165641000
1 1.399538000 1.500253000 -1.999234000
5 -0.342347000 -0.395474000 -1.598017000
1 -0.596822000 -0.649443000 -2.737266000

[B₁₂H₁₂]_{-ap}_MeCN E = -305.041477377 Ha

5 -0.665172000 -0.795516000 1.001263000
5 0.400289000 0.347911000 1.639712000
1 0.616184000 0.56001000 2.785244000
5 0.969320000 -1.190056000 0.853855000
1 1.565210000 -2.004745000 1.474388000
5 -0.272381000 -1.684100000 -0.379361000
1 -0.504767000 -2.828198000 -0.581435000
5 -1.193141000 0.804536000 0.892308000
1 -2.040949000 1.321794000 1.538348000
5 -1.609006000 -0.451455000 -0.355601000
1 -2.734217000 -0.772060000 -0.541981000
5 1.216729000 -0.848031000 -0.872869000
1 2.057243000 -1.419698000 -1.489139000
5 1.624857000 0.384097000 0.351487000
1 2.751405000 0.676031000 0.593284000
5 -0.905027000 1.108934000 -0.835470000
1 -1.553275000 1.911275000 -1.426298000
5 0.313413000 1.593899000 0.374545000
1 0.519367000 2.735955000 0.631736000
5 0.815688000 0.851423000 -1.149265000
1 1.386251000 1.484853000 -1.978529000
5 -0.346616000 -0.399923000 -1.606502000
1 -0.602852000 -0.656229000 -2.738511000

[B₁₃H₁₃]²⁻_MeCN E = -331.205624141 Ha

5 0.073777000 1.445963000 0.698923000
5 -0.036353000 -1.195234000 0.841157000
1 -1.343146000 0.206872000 1.233446000
5 1.400691000 0.090006000 1.175126000
1 0.131350000 2.557281000 1.141486000
1 -0.070231000 -2.252407000 1.402637000
5 0.048514000 0.193062000 2.049130000
5 -1.456770000 1.003726000 0.342533000
5 -1.529078000 -0.742034000 -0.248322000
5 1.443220000 -0.869174000 -0.311538000
5 1.515573000 0.876402000 -0.405823000
5 0.034868000 1.440298000 -1.126242000
5 -0.082070000 -1.382331000 -0.974230000

5 0.841936000 -0.043274000 -1.719192000
5 -0.920057000 0.032255000 -1.681392000
1 0.076178000 0.255968000 3.239098000
1 -2.357707000 0.281805000 1.869641000
1 2.442718000 0.078356000 1.769649000
1 -2.415988000 1.710368000 -0.431751000
1 -2.543468000 -1.372928000 -0.266763000
1 2.399057000 -1.583428000 -0.371020000
1 2.527055000 1.498220000 -0.536848000
1 0.066358000 2.471715000 -1.727482000
1 -0.140993000 -2.471887000 -1.459238000
1 1.399300000 -0.123831000 -2.771270000
1 -1.526827000 0.001881000 -2.708785000

[B₁₃H₁₃]_{-ap}_MeCN E = -330.475236632 Ha

5 0.362162000 1.549611000 0.556191000
5 0.242430000 -1.337579000 0.712587000
5 -2.005852000 0.251143000 1.465760000
1 1.258409000 0.090703000 1.080694000
1 0.423353000 2.586982000 1.130376000
1 0.221047000 -2.309185000 1.394903000
5 -0.474509000 0.173729000 1.290746000
5 -1.206016000 1.014461000 -0.130575000
5 -1.279704000 -0.752471000 -0.035080000
5 1.555639000 -0.889512000 -0.365672000
5 1.629027000 0.881817000 -0.461637000
5 0.119322000 1.459305000 -1.200993000
5 0.000335000 -1.416549000 -1.045133000
5 0.849450000 -0.046488000 -1.772727000
5 -0.900266000 0.036161000 -1.579880000
1 -3.143842000 0.311797000 1.727787000
1 1.997813000 1.010452000 2.010176000
1 -2.212853000 1.653036000 0.028729000
1 -2.334260000 -1.286783000 0.184487000
1 2.534285000 -1.558056000 -0.463247000
1 2.658980000 1.452493000 -0.626847000
1 0.054646000 2.447153000 -1.857184000
1 -0.149161000 -2.460567000 -1.591035000
1 1.347534000 -0.126936000 -2.849744000
1 -1.646238000 0.016964000 -2.504002000

[B₁₃H₁₃]_{-eq1}_MeCN E = -330.475227695 Ha

5 -0.006962000 1.690303000 0.390194000
5 -0.143896000 -1.175351000 0.733684000
5 -0.974824000 0.348801000 1.083971000
5 0.829648000 0.300915000 1.098811000
1 0.009975000 2.741271000 0.942197000
1 -0.180901000 -2.066304000 1.539891000
5 0.284793000 -0.288300000 2.165688000
5 -1.45529000 1.086162000 -0.440683000
5 -1.552774000 -0.690440000 -0.232604000
5 1.351575000 -0.799926000 -0.184256000
5 1.436558000 0.976996000 -0.394095000
5 0.024606000 1.460028000 -1.351213000
5 -0.102790000 -1.394347000 -1.013232000
5 0.857785000 -0.067868000 -1.703713000
5 -0.926660000 -0.003082000 -1.729524000
1 -0.018187000 -0.699007000 3.468881000
1 -1.559357000 0.470712000 2.128331000
1 -2.440588000 1.746876000 -0.502922000
1 -2.589011000 -1.268540000 -0.179631000
1 2.312877000 -1.480651000 -0.035199000
1 2.473881000 1.553942000 -0.438301000
1 0.076143000 2.382970000 -2.099299000
1 -0.133267000 -2.486165000 -1.479699000
1 1.491645000 -0.213761000 -2.699134000
1 -1.529549000 -0.095939000 -2.750609000

[B₁₃H₁₃]_{-eq2}_MeCN E = -330.475267460 Ha

5 -0.342460000 1.747573000 0.518099000
5 -0.170567000 -1.094640000 0.836327000

5 -1.201489000 0.313579000 1.161877000
5 1.710925000 -1.121263000 1.338898000
1 -0.445470000 2.806235000 1.046284000
1 -0.084216000 -2.030923000 1.586121000
5 0.563527000 0.451683000 1.293113000
5 -1.645495000 0.987422000 -0.404089000
5 -1.537181000 -0.768478000 -0.225169000
5 1.309165000 -0.527543000 -0.252959000
5 1.201039000 1.231009000 -0.192038000
5 -0.171944000 1.551512000 -1.240541000
5 0.001442000 -1.295297000 -0.938429000
5 0.854870000 1.045560000 -1.574170000
5 -0.907754000 0.002017000 -1.698245000
1 1.137392000 0.542321000 2.345973000
1 -1.917157000 0.373349000 2.108136000
1 2.122772000 -1.605802000 2.200118000
1 -2.690560000 1.531364000 -0.567479000
1 -2.483349000 -1.486528000 -0.221655000
1 2.180416000 1.899064000 -0.125507000
1 -0.188373000 2.487767000 -1.973616000
1 0.146094000 -2.383793000 -1.389987000
1 1.576430000 0.081430000 -2.515622000
1 -1.439208000 -0.146489000 -2.751496000

[B₁₃H₁₃]_{-eq3}_MeCN E = -330.422095391 Ha

5 0.072530000 1.420465000 0.688861000
5 -0.025770000 -0.886278000 0.714993000
5 -1.366758000 0.199567000 1.246656000
5 1.423938000 0.082024000 1.187068000
1 0.129869000 2.497174000 1.193866000
5 0.048241000 0.181347000 2.069290000
5 -1.467584000 1.000136000 -0.363783000
5 -1.556819000 -0.744029000 -0.275796000
5 1.468878000 -0.873501000 -0.339857000
5 1.525604000 0.871950000 -0.427604000
5 0.034417000 1.429672000 -1.129881000
5 -0.082603000 -1.380149000 -0.984870000
5 0.845354000 -0.046485000 -1.739597000
5 -0.924694000 0.029371000 -1.701965000
1 0.076159000 0.240334000 3.240373000
1 -2.369324000 0.275650000 1.877338000
1 2.454217000 0.073175000 1.776121000
1 -2.421898000 1.707623000 -0.402424000
1 -2.533698000 -1.415155000 -0.252482000
1 2.384895000 -1.625584000 -0.355165000
1 2.534459000 1.494971000 -0.508625000
1 0.067551000 2.474380000 -1.695965000
1 -0.139320000 -2.499306000 -1.375121000
1 1.394774000 -0.136429000 -2.788870000
1 -1.524281000 -0.010866000 -2.726716000

[B₁₃H₁₃]_{-eq4}_MeCN E = -330.408317226 Ha

5 0.100453000 1.445505000 0.715793000
5 -0.009612000 -1.195024000 0.857997000
5 -1.398422000 0.209722000 1.240580000
5 1.377209000 0.089156000 1.145374000
1 0.144878000 2.556436000 1.144863000
1 -0.056386000 -2.252606000 1.405065000
5 0.012786000 0.193581000 2.029154000
5 -1.480179000 1.026077000 -0.328392000
5 -1.554011000 -0.761026000 -0.232098000
5 1.463997000 -0.882769000 -0.332436000
5 1.537469000 0.885753000 -0.427915000
5 0.062590000 1.481199000 -1.110258000
5 -0.057908000 -1.423607000 -0.953812000
5 0.859479000 -0.045651000 -1.750446000
5 -0.784055000 0.038506000 -1.0385634000
1 0.058614000 0.255356000 3.214236000
1 -2.403171000 0.284744000 1.882531000
1 2.404232000 0.079006000 1.753852000
1 -2.405580000 1.750482000 -0.482700000

1 -2.537070000 -1.418534000 -0.310871000
1 2.427985000 -1.576602000 -0.389588000
1 2.555342000 1.486781000 -0.555341000
1 0.014756000 2.489847000 -1.729912000
1 -0.192695000 -2.485694000 -1.461054000
1 1.364030000 -0.124868000 -2.819340000

[B_{1s}H_{1s}]²_MeCN E = -356.701323224 Ha

5 -1.703558000 -0.346995000 0.756726000
5 -1.130911000 1.287220000 0.748512000
5 0.570489000 1.608807000 0.745957000
5 1.699534000 0.296090000 0.752094000
5 1.126910000 -1.338141000 0.760271000
5 -0.574488000 -1.659732000 0.762274000
1 -1.805104000 2.074623000 1.341142000
1 0.912678000 2.588207000 1.336770000
1 2.716657000 0.490702000 1.346041000
1 1.801744000 -2.119532000 1.360083000
1 -0.916202000 -2.633483000 1.362603000
1 -2.720228000 -0.535739000 1.353349000
5 -1.636980000 0.539724000 -0.756877000
5 -0.324212000 1.668755000 -0.763191000
5 1.310041000 1.096159000 -0.761125000
5 1.631624000 -0.605236000 -0.752743000
5 0.318886000 -1.734263000 -0.747023000
5 -1.315361000 -1.161629000 -0.749056000
1 -0.516264000 2.682736000 -1.363320000
1 2.094233000 1.767696000 -1.361003000
1 2.607964000 -0.950011000 -1.347106000
1 0.510224000 -2.754059000 -1.337446000
1 -2.099984000 -1.839059000 -1.341666000
1 -2.613801000 0.878926000 -1.353640000
5 -0.002999000 -0.036601000 -1.547043000
5 -0.001674000 -0.021576000 1.546337000
1 -0.003494000 -0.042418000 -2.742457000
1 -0.001177000 -0.015737000 2.741751000

[B_{1s}H_{1s}]²_ap_MeCN E = -355.905634542 Ha

5 -1.707150000 -0.347471000 0.761079000
5 -1.133306000 1.289985000 0.753142000
5 0.571738000 1.612127000 0.751051000
5 1.703120000 0.296632000 0.756446000
5 1.129304000 -1.340051000 0.764920000
5 -0.575742000 -1.668291000 0.767419000
1 -1.812036000 2.082567000 1.321946000
1 0.915936000 2.597703000 1.319001000
1 2.727142000 0.492269000 1.326739000
1 1.808596000 -2.127788000 1.340846000
1 -0.919509000 -2.643023000 1.345007000
1 -2.730693000 -0.537551000 1.334097000
5 -1.654878000 0.546042000 -0.757701000
5 -0.327562000 1.688124000 -0.763420000
5 1.324800000 1.109125000 -0.761520000
5 1.649520000 -0.611547000 -0.753548000
5 0.322253000 -1.753651000 -0.747009000
5 -1.330098000 -1.174628000 -0.749290000
1 -0.514129000 2.669682000 -1.399869000
1 2.084043000 1.759280000 -1.397505000
1 2.594962000 -0.945829000 -1.384394000
1 0.508148000 -2.741396000 -1.374007000
1 -2.089865000 -1.830869000 -1.378356000
1 -2.600851000 0.874291000 -1.390906000
5 -0.002872000 -0.035117000 -1.251724000
5 -0.001677000 -0.021551000 1.555299000
1 -0.001152000 -0.015789000 2.744927000

[B_{1s}H_{1s}]²_eq_MeCN E = -355.910791002 Ha

5 -1.736293000 -0.353336000 0.767447000
5 -1.138884000 1.292806000 0.760109000
5 0.571118000 1.610448000 0.744863000
5 1.708920000 0.295198000 0.763971000

5 1.148243000 -1.363785000 0.771373000
5 -0.488151000 -1.413339000 0.630884000
1 -1.814410000 2.068872000 1.354368000
1 0.912680000 2.588409000 1.328329000
1 2.720192000 0.480351000 1.359356000
1 1.749433000 -2.146464000 1.428729000
1 -2.695392000 -0.589950000 1.423295000
5 -1.675794000 0.540254000 -0.755741000
5 -0.334813000 1.648965000 -0.761081000
5 1.306179000 -1.073969000 -0.758940000
5 1.662061000 -0.629124000 -0.751235000
5 0.343635000 -1.740151000 -0.790004000
5 -1.338773000 -1.150906000 -0.792394000
1 -0.536133000 2.654593000 -1.363471000
1 2.092498000 1.733161000 -1.360827000
1 2.645430000 -0.954022000 -1.334401000
1 0.442805000 -2.771743000 -1.361728000
1 -2.058382000 -1.895829000 -1.365321000
1 -2.645576000 0.899362000 -1.341561000
5 0.005628000 -0.011299000 -1.552224000
5 0.017950000 0.034825000 -1.570180000
1 -0.007109000 -0.052613000 -2.741299000
1 -0.006312000 -0.029741000 2.754936000

[B_{1s}H_{1s}]²_MeCN E = -382.136137414 Ha

5 0.017219000 6.759286000 13.091669000
5 -0.285927000 5.468433000 12.006638000
1 -1.157242000 5.474040000 11.194263000
5 1.156193000 6.383109000 11.868333000
1 1.404191000 7.098372000 10.947960000
5 -0.717032000 5.287178000 13.695590000
5 1.214316000 4.649165000 11.620255000
1 1.333045000 4.289619000 10.488234000
5 1.728300000 6.838118000 13.460659000
1 2.189266000 7.935159000 13.554399000
5 0.146032000 3.819982000 12.915390000
5 2.581436000 5.364531000 12.681459000
1 3.621448000 5.581638000 12.133488000
5 0.657849000 5.999845000 14.748898000
1 0.321213000 6.670795000 15.679227000
5 1.987141000 3.588355000 12.666040000
1 2.497094000 2.693749000 12.062277000
5 2.501523000 5.777596000 14.056626000
1 3.353484000 6.339930000 15.125442000
5 0.055932000 4.225851000 14.740730000
1 -0.719967000 3.755939000 15.516579000
5 2.821165000 4.098552000 14.120405000
1 3.908650000 3.660941000 14.334868000
5 1.682575000 4.474306000 15.344130000
1 1.886615000 4.327679000 16.509112000
5 1.379341000 3.183610000 14.259134000
1 1.348680000 2.036916000 14.581960000
1 -0.619245000 7.766557000 13.120560000
1 -1.882963000 5.351412000 13.943382000
1 -0.556992000 2.931439000 12.534047000

[B_{1s}H_{1s}]²_ap_MeCN E = -381.332291945 Ha

5 0.016173000 6.744856000 13.097520000
5 -0.289883000 5.456125000 12.006682000
1 -1.157101000 5.469802000 11.195818000
5 1.157261000 6.368030000 11.871757000
1 1.396989000 7.082380000 10.952974000
5 -0.747495000 5.286464000 13.700345000
1 2.125087000 4.638224000 11.591327000
5 1.330893000 2.493241000 10.459530000
1 1.730801000 6.826118000 13.466586000
1 2.188826000 7.92067000 13.557707000
5 0.112245000 3.821051000 12.883548000
5 2.595979000 5.373854000 12.675483000
1 3.635144000 5.577127000 12.132847000
5 0.656749000 6.014561000 14.759822000

1 0.320977000 6.671124000 15.693517000
5 2.008606000 3.581918000 12.620698000
1 2.517177000 2.645040000 12.100819000
5 2.522292000 5.792318000 14.521486000
1 3.371763000 6.347098000 15.140921000
5 0.013630000 4.240714000 14.764157000
1 -0.694258000 3.705311000 15.550831000
5 2.859525000 4.114138000 14.124100000
1 3.897797000 3.598060000 14.352869000
5 1.695295000 4.498214000 15.375395000
1 1.883026000 4.262502000 16.518183000
5 1.347511000 3.462681000 14.143601000
1 -0.620390000 7.748098000 13.118800000
1 -1.909299000 5.363049000 13.940711000
1 -0.550660000 2.892481000 12.551760000

[B_{1s}H_{1s}]²_eq_MeCN E = -381.346494683 Ha

5 0.009782000 6.773570000 13.110191000
5 -0.299755000 5.487739000 12.000180000
1 -1.172901000 5.507136000 11.197442000
5 1.143262000 6.403279000 11.861745000
1 1.380681000 7.127263000 10.952226000
5 -0.738237000 5.271381000 13.676298000
5 1.208138000 4.659607000 11.624491000
1 1.325268000 4.304110000 10.496025000
5 1.748620000 6.848472000 13.437400000
1 2.214709000 7.926945000 13.580990000
5 0.159350000 5.1811237000 12.896628000
5 2.581301000 5.346967000 12.663659000
1 3.621846000 5.588319000 12.139475000
5 0.747680000 5.820314000 14.500152000
5 1.987387000 3.590597000 12.678632000
1 2.496226000 2.698389000 12.079749000
5 2.532509000 5.772810000 14.498064000
1 3.346972000 6.373880000 15.111519000
5 0.045939000 4.195796000 14.736693000
1 -0.750154000 3.774560000 15.504594000
5 2.829489000 4.089821000 14.142269000
1 3.909853000 3.656529000 14.372127000
5 0.167630600 4.487048000 15.364050000
1 1.845648000 4.396906000 16.532481000
5 1.386377000 3.174484000 14.280634000
1 1.356432000 2.037299000 14.617517000
1 -0.616036000 7.774422000 13.203116000
1 -1.882537000 5.328028000 13.973337000
1 -0.562026000 2.934397000 12.540845000

[B_{1s}H_{1s}]²_eq2_MeCN E = -381.353257646 Ha

5 0.003083000 6.780251000 13.097129000
5 -0.305931000 5.464078000 11.990751000
1 -1.174920000 5.486385000 11.184075000
5 1.1422695000 6.384717000 11.870190000
1 1.373485000 7.102423000 10.952374000
5 -0.715974000 5.286277000 13.695902000
5 1.217401000 4.657731000 11.608734000
1 1.353957000 4.292977000 10.486031000
5 1.731577000 6.846949000 13.449468000
1 2.208007000 7.931264000 13.546438000
5 0.131136000 3.833788000 12.835551000
5 2.570690000 5.360738000 12.689015000
1 3.617315000 5.560936000 12.159429000
5 0.658033000 6.078701000 14.727302000
1 0.323784000 6.663752000 15.698787000
5 1.978999000 3.588613000 12.673788000
1 2.455126000 2.672690000 12.084221000
5 2.492004000 5.771991000 14.509633000
1 3.314700000 6.332183000 15.159707000
5 0.278315000 4.354372000 14.527969000
5 2.836504000 4.071911000 14.147685000
1 3.937105000 3.665135000 14.322821000
5 1.713075000 4.434728000 15.390229000

1 1.815550000 4.398681000 16.567174000
5 1.407656000 3.136803000 14.298004000
1 1.248808000 1.991126000 14.541524000
1 -0.637276000 7.778706000 13.110528000
1 -1.843916000 5.235729000 14.070424000
1 -0.557062000 2.912528000 12.545026000

[B_{1s}H_{1s}]²_MeCN E = -407.597844685 Ha

5 0.138251000 1.280422000 0.932762000
5 -0.872345000 -1.447266000 1.497525000
5 -1.414882000 0.245570000 1.106670000
5 1.546487000 0.157171000 1.269131000
1 0.025763000 2.354728000 1.442159000
5 -1.291157000 -2.181447000 2.338340000
5 0.022480000 -0.074605000 2.047255000
5 -1.606656000 0.333569000 -0.753226000
5 -1.921806000 1.133949000 0.161533000
5 0.848665000 -1.445043000 1.170579000
5 1.505972000 1.123977000 -0.160277000
5 -0.044761000 1.356443000 -0.931296000
5 0.544445000 -1.355536000 -1.474797000
5 1.225084000 0.252060000 -1.625448000
5 -1.204203000 -1.336272000 -1.395328000
1 -0.005220000 1.48178000 3.218279000
1 -2.28947000 0.807921000 1.693672000
1 2.482060000 0.327520000 1.988642000
1 -2.583764000 0.936325000 -1.082178000
1 -3.047561000 -1.512157000 0.267863000
1 1.465789000 -2.301054000 1.729532000
1 2.302398000 2.009579000 -0.211120000
1 -0.249822000 2.459941000 -1.338177000
1 1.009636000 -2.169728000 -2.213832000
1 1.980676000 0.467404000 -2.522436000
1 -1.815947000 -2.007458000 -2.168160000
5 -0.441555000 0.069658000 -2.045151000
1 -0.746288000 0.359426000 -3.160921000
5 1.796523000 -0.678212000 -0.251863000
1 2.881331000 -1.157791000 -3.90328000
5 -0.401613000 -2.125238000 -0.051048000
1 -0.401151000 -3.318737000 -0.094192000

[B_{1s}H_{1s}]²_ap_MeCN E = -406.809772083 Ha

5 0.138089000 1.288703000 0.926475000
5 -0.896431000 -1.4273928000 1.489558000
5 -1.422394000 0.250460000 1.098913000
5 1.580003000 0.166740000 1.257520000
1 0.051527000 2.342336000 1.470986000
1 -1.172371000 -2.173675000 2.402852000
5 0.020943000 -0.077577000 2.003707000
5 -1.614715000 0.328183000 -0.755930000
5 -1.974876000 -1.145561000 0.166160000
5 0.670244000 -1.229613000 0.782913000
5 1.538623000 1.167247000 -0.162976000
5 -0.041215000 1.359355000 -0.927065000
5 0.556932000 -1.353796000 -1.331706000
5 1.243152000 0.279841000 -1.627074000
5 -1.236416000 -1.342880000 -1.394128000
1 0.052311000 0.056776000 3.178425000
1 -2.282826000 0.787667000 1.718985000
1 2.439825000 0.6289015000 2.067864000
1 -2.584540000 0.933802000 -1.084764000
1 -3.104446000 -1.491056000 0.282911000
1 2.307738000 2.070435000 -0.202601000
1 -0.252046000 2.457237000 -1.333490000
1 1.061459000 -2.213418000 -1.977698000
1 1.952084000 0.454847000 -2.562922000
1 -1.797469000 1.595730000 -2.213876000
5 -0.427056000 0.050750000 -2.015786000
1 -0.703205000 0.300658000 -3.144141000
5 1.920728000 -0.582459000 -0.275828000
1 2.970109000 -1.113415000 -0.415900000

5 -0.541287000 -2.201981000 -0.051029000
1 -0.480900000 -3.383492000 -0.105720000

[B₁₆H₁₆]_{eq}_MeCN E = -406.80978763 Ha

5 0.154106000 1.290249000 0.959400000
5 -0.877958000 -1.430358000 1.523313000
5 -1.399584000 0.264955000 1.089856000
5 1.557810000 0.140226000 1.304621000
1 0.094846000 2.359839000 1.475110000
1 -1.331943000 2.315094000 2.315094000
5 0.023123000 -0.059787000 2.096581000
5 -1.625617000 0.318035000 -0.784808000
5 -1.887450000 -1.132417000 0.152907000
5 0.848986000 -1.449235000 1.318148000
5 1.473622000 1.100035000 -0.153423000
5 -0.076424000 1.348413000 -0.907726000
5 0.513595000 -1.348588000 -1.616383000
5 1.213550000 0.244428000 -1.653043000
5 -1.216374000 -1.334678000 -1.428354000
1 -0.025786000 0.181709000 3.257707000
1 -2.272527000 0.833296000 1.664710000
1 2.574943000 0.317533000 1.882290000
1 -2.603306000 0.911859000 -1.111260000
1 -2.991899000 -1.554889000 0.269868000
1 1.467601000 -2.328902000 1.814332000
1 2.334085000 1.907850000 -0.229539000
1 -0.245531000 2.450829000 -1.320264000
1 0.999580000 -2.185856000 -2.298707000
1 2.071644000 0.473726000 -2.444770000
1 -1.841219000 -0.245610000 -2.144729000
5 -0.460223000 0.081615000 -2.092259000
1 -0.760031000 0.406834000 -3.193793000
5 1.330112000 -0.693259000 -0.199845000
5 -0.297038000 -2.046849000 -0.059420000
1 -0.188664000 -3.228504000 -0.111123000

[B₁₇H₁₇]²⁺_MeCN E = -433.066183332 Ha

5 0.295705000 1.411782000 0.841571000
5 -1.160099000 -1.700370000 1.205659000
5 -2.091790000 -0.361666000 0.593746000
5 1.226887000 0.072755000 1.453634000
1 0.154655000 2.414401000 1.468843000
1 -1.488292000 -2.295034000 2.184042000
5 -0.582685000 -0.013704000 1.537143000
5 -1.142413000 0.978924000 -0.174565000
5 -2.037225000 -1.863071000 -0.295086000
5 0.636563000 -1.578948000 0.994082000
5 1.826288000 1.007000000 0.106181000
5 0.459634000 1.433537000 -0.892612000
5 0.830254000 -1.553660000 -1.052870000
5 1.492057000 0.107634000 -1.352157000
5 -1.927973000 -0.339701000 -1.140528000
1 -0.908253000 0.269324000 2.653584000
1 -3.088251000 0.004537000 1.133820000
1 1.754389000 0.113738000 2.520637000
1 -1.851847000 1.941636000 -0.229669000
1 -2.988572000 -2.570688000 -0.393137000
1 1.143798000 -2.366722000 1.738818000
1 2.777785000 1.714379000 0.204349000
1 0.435662000 2.451265000 -1.511149000
1 1.470409000 -2.323177000 -1.709282000
1 2.209852000 0.172820000 -2.300632000
1 -2.806875000 0.043397000 -1.847110000
5 -0.269298000 0.027478000 -1.775123000
1 -0.380971000 0.338480000 -2.925520000
5 1.966119000 -0.732906000 0.097755000
1 3.024043000 -1.271727000 0.192136000
5 -0.420950000 -2.506220000 -0.150351000
1 -0.217256000 -3.679796000 -0.145956000
5 -0.894933000 -1.665182000 -1.600143000

1 -1.031813000 -2.234020000 -2.637507000

[B₁₇H₁₆]_{ap1}_MeCN E = -432.253630078 Ha

5 0.281269000 1.404855000 0.842328000
5 -1.135740000 -1.696897000 1.249090000
5 -2.094378000 -0.318829000 0.619291000
5 1.214846000 0.062585000 1.455716000
1 0.144734000 2.406013000 1.467289000
1 -1.530424000 -2.323674000 2.171686000
5 -0.590510000 -0.001210000 1.582172000
5 -1.167643000 1.023429000 -0.175227000
5 -1.807887000 -1.692778000 -0.271445000
5 0.662577000 -1.608157000 1.025906000
5 1.807895000 0.993261000 0.104079000
5 0.444833000 1.426300000 -0.895626000
5 0.862144000 -1.582294000 -1.080085000
5 1.479130000 0.096344000 -1.356142000
5 -1.925283000 -0.295522000 -1.165264000
1 -0.918373000 0.279795000 2.692989000
1 -3.125129000 -0.031558000 1.124228000
1 1.743656000 0.106736000 2.518661000
1 -1.877413000 1.978955000 -0.230006000
1 1.163322000 -2.394027000 1.168238000
1 2.757262000 1.698795000 0.201006000
1 0.425859000 2.442056000 -1.511859000
1 1.495949000 -2.351751000 -1.732600000
1 2.197991000 0.164318000 -2.299944000
1 -2.844226000 0.006389000 -1.846583000
5 -0.269585000 0.045243000 -1.822660000
1 -0.384121000 0.352055000 -2.968182000
5 1.955135000 -0.745504000 0.096796000
1 3.012944000 -1.278160000 0.190647000
5 -0.374515000 -2.525699000 -1.462940000
1 -0.263752000 -3.703636000 -0.150715000
5 -0.861783000 -1.659332000 -1.638274000
1 -1.075608000 -2.262249000 -2.633510000

[B₁₇H₁₆]_{ap2}_MeCN E = -432.262818236 Ha

5 0.296551000 1.427786000 0.890699000
5 -1.163799000 -1.696129000 1.249090000
5 -2.111621000 -0.364344000 0.590081000
5 1.241704000 0.075868000 1.465183000
1 0.164781000 2.461156000 1.446618000
1 -1.488944000 -2.289001000 2.178973000
5 -0.586831000 -0.017320000 1.549573000
5 -1.182540000 0.976202000 -0.156745000
5 -2.044434000 -1.865642000 -0.297669000
5 0.634924000 -1.566652000 0.985966000
5 1.853199000 1.012971000 0.116895000
5 0.417563000 1.151418000 -0.748184000
5 0.835349000 -1.567701000 -1.055746000
5 1.531088000 0.080931000 -1.373593000
5 -1.954161000 -0.349643000 -1.148894000
1 -0.917500000 0.280415000 2.655030000
1 -3.098794000 0.012275000 1.131419000
1 1.767783000 0.121568000 2.527335000
1 -1.805440000 1.985848000 -0.263799000
1 -2.986330000 -2.581739000 -0.385613000
1 1.149190000 -2.344607000 1.729490000
1 2.758185000 1.771071000 0.159174000
1 1.470943000 -2.323554000 -1.722787000
1 2.219774000 0.219616000 -2.322777000
1 -2.814297000 0.056243000 -1.859192000
5 -0.284705000 -0.001554000 -1.803416000
1 -0.358067000 0.409715000 -2.919090000
5 1.984836000 -0.734310000 0.103198000
1 3.041017000 -1.266438000 0.194432000
5 -0.423548000 -2.502856000 -0.155239000
1 -0.219354000 -3.672958000 -0.149782000

5 -0.910638000 -1.671451000 -1.610774000
1 -1.036942000 -2.231953000 -2.649525000

[B₁₇H₁₆]_{eq}_MeCN E = -432.297950034 Ha

5 0.278847000 1.416636000 0.863112000
5 -1.157226000 -1.693232000 1.232016000
5 -2.094014000 -0.346241000 0.616358000
5 1.215369000 0.069580000 1.478729000
1 0.005155000 2.380649000 1.491369000
1 -1.368850000 -2.236247000 2.261286000
5 -0.478613000 -0.104107000 1.182350000
5 -1.112368000 0.950260000 -0.255366000
5 -2.062795000 -1.866202000 -0.263047000
5 0.656355000 -1.593338000 0.906443000
5 1.832143000 1.027278000 0.141564000
5 0.488891000 1.448563000 -0.901997000
5 0.825893000 -1.549411000 -1.042295000
5 1.512621000 0.128468000 -1.338862000
5 -1.948689000 -0.362120000 -1.154976000
1 -3.017611000 0.134598000 1.177473000
1 1.654320000 0.009147000 2.575440000
1 -1.819996000 1.903305000 -0.260074000
1 -3.012342000 -2.569008000 -0.354144000
1 1.138012000 -2.350472000 1.683418000
1 2.778054000 1.733195000 0.245333000
1 0.449240000 2.479229000 -1.486208000
1 1.464213000 -2.317470000 -1.828555000
1 2.236933000 0.202851000 -2.275894000
1 -2.840447000 0.035792000 -1.826956000
5 -0.271698000 0.028916000 -1.763659000
1 -0.384940000 0.341241000 -2.908727000
5 1.994589000 -0.716681000 0.087787000
1 3.044328000 -1.251087000 0.220041000
5 -0.442922000 -2.527473000 -0.165602000
1 -0.245704000 -3.695551000 -0.121804000
5 -0.922234000 -1.680338000 -1.591845000
1 -1.071656000 -2.25358000 -2.619840000

[Li₂B₂H₂]_{MeCN} E = -65.9199338927 Ha

5 0.121911000 0.018464000 -0.038680000
5 1.371085000 -0.130635000 -0.761327000
1 2.392998000 -0.244212000 -1.354863000
1 -0.900539000 0.137897000 0.552737000
3 -0.370130000 -0.496174000 -2.220135000
3 1.837238000 0.747313000 1.309495000

[Li₂B₂H₂]⁺_MeCN E = -65.1026054635 Ha

5 -0.132362000 -0.234811000 -0.000214000
5 1.008839000 0.834432000 -0.140313000
1 1.823222000 1.674776000 -0.253650000
3 -1.798416000 -1.715929000 0.197637000
3 1.671962000 -1.707890000 0.259376000

[Li₂B₃H₃]_{MeCN} E = -91.3972239722 Ha

5 4.245291000 1.130537000 1.473249000
5 4.102352000 1.046832000 -0.093805000
5 2.807473000 0.964576000 0.821446000
1 1.609020000 0.855146000 0.934919000
1 4.886310000 1.239341000 2.847326000
1 4.549974000 1.033707000 -1.211942000
3 2.698496000 1.073903000 3.060262000
3 2.295339000 0.795300000 1.355652000

[Li₂B₃H₃]⁺_MeCN E = -90.6315938884 Ha

5 4.258771000 1.127470000 1.567331000
5 4.097753000 1.045403000 -0.186192000
5 2.990160000 0.965714000 0.805263000
1 5.202697000 1.245977000 2.261013000
1 4.897886000 1.087793000 -1.048753000
3 2.264479000 1.063361000 3.038398000
3 1.873488000 0.748478000 -1.256175000

[Li₂B₄H₄]_{MeCN} E = -116.843807351 Ha

5 2.486946000 0.147439000 2.319492000
5 2.837920000 0.838554000 0.931855000
1 3.056211000 1.912447000 0.430380000
5 2.507913000 -0.675428000 0.495329000
5 3.552871000 -0.872517000 1.676112000
1 1.903395000 0.335317000 3.357070000
1 1.919378000 -1.276117000 -0.367756000
1 4.505682000 -1.533841000 2.003768000
3 2.128295000 2.334978000 2.408609000
3 3.555932000 -2.624917000 0.317833000

[Li₂B₄H₃]⁺_MeCN E = -116.110132545 Ha

5 2.592793000 0.199981000 2.653051000
5 2.571101000 0.637704000 1.053582000
1 2.431485000 1.676728000 0.482380000
5 2.812187000 -0.708596000 0.079686000
5 2.789021000 -0.901630000 1.598778000
1 2.494884000 0.664807000 3.738140000
1 2.872594000 -0.931581000 -1.074776000
3 2.234034000 2.519866000 2.415390000
3 3.150762000 -3.037524000 0.622693000

[Li₂B₅H₅]_{MeCN} E = -142.336473283 Ha

5 4.469625000 -1.152196000 0.777111000
5 5.039239000 -1.300549000 -0.745829000
5 2.953647000 -0.458975000 0.548701000
5 3.386387000 -1.563913000 -0.572609000
5 4.131260000 0.059774000 -0.493746000
1 2.779653000 -2.403688000 -1.187747000
1 4.917086000 -1.434783000 1.859698000
1 4.287542000 1.153028000 -0.950934000
1 2.010647000 -0.089102000 1.183163000
3 1.200425000 -1.703613000 -0.104618000
1 5.973614000 -1.725554000 -1.358183000
3 6.480356000 -2.175195000 0.708538000

[Li₂B₅H₄]_{ap}_MeCN E = -141.510542071 Ha

5 4.634912000 -1.239912000 0.880843000
5 4.864620000 -1.379376000 -0.652739000
5 2.996762000 -0.780697000 0.640131000
5 3.316136000 -2.072151000 -0.165626000
5 3.929290000 0.068539000 -0.289329000
1 2.932076000 -3.023424000 -0.753699000
1 5.164431000 -1.342977000 1.951264000
1 4.097714000 1.023845000 -0.944695000
3 1.525175000 -0.490453000 -1.091503000
1 5.371127000 -1.574554000 -1.704354000
3 6.786592000 -1.894504000 0.680090000

[Li₂B₅H₄]_{eq}_MeCN E = -141.544416029 Ha

5 4.454428000 -1.425281000 0.724039000
5 5.077446000 -1.359928000 -0.731799000
5 2.733508000 -0.307406000 0.278705000
5 3.405180000 -1.346953000 -0.576045000
5 4.196739000 0.082973000 -0.548198000
1 4.518373000 -1.573892000 1.897356000
1 4.556942000 1.201235000 -0.653735000
1 1.991257000 0.255258000 0.999325000
3 1.244561000 -2.116239000 0.372653000
1 5.919300000 -1.760699000 -1.470592000
3 6.752093000 -2.040145000 0.629583000

[Li₂B₅H₃]_{conf1}_MeCN E = -167.851881979 Ha

3 1.539542000 1.578435000 1.723381000
5 1.292672000 0.042367000 -0.001054000
1 2.479497000 1.802510000 0.090667000
5 -0.022828000 1.168837000 0.034903000
5 0.038220000 -0.128708000 1.181508000
5 0.124794000 0.048409000 -1.240945000
5 -1.129661000 -0.122624000 -0.058385000
5 0.185857000 -1.249063000 -0.094308000
1 -2.316527000 -0.260504000 -0.150022000

1	0.11395000	0.07617400	-2.43862200
1	0.23380100	-2.44008700	-0.21619000
1	0.04903700	-0.15648400	2.37908700
1	-0.07076500	2.35974800	0.15681700
3	-1.37625800	-1.65891700	-1.78286300

{Li2[BaHs]}* _conf1_MeCN E = -167.044102828 Ha

3	1.45635000	1.44302500	2.07468400
5	1.41037700	0.10134100	-0.02057100
1	2.57817000	0.21307900	0.13360900
5	0.01919200	1.29780300	0.01436400
5	0.05176000	-0.10092000	0.99607900
5	0.23458500	0.17322900	-1.13297700
5	-1.11749400	-0.05206800	-0.22940900
5	0.24206200	-1.21974100	-0.26314000
1	-2.29275500	-0.17269200	-0.34749200
1	0.29816700	-2.39661400	-0.41040200
1	-0.02892100	-0.22970800	2.17927500
1	-0.04613600	2.46499500	0.19533100
3	-1.77797800	-2.16006700	-1.16675600

Li2[BaHs]_conf0_MeCN E = -167.857182107 Ha

3	1.70175800	1.64326300	1.62878200
5	1.21480500	-0.01334500	0.09546000
1	2.41211500	0.02778900	0.14604500
5	0.00037300	1.21986800	0.13371400
5	-0.00094100	-0.03332900	1.31448700
5	0.00558900	0.04914500	-1.12225500
5	-1.21009000	0.02948400	0.09074900
5	0.00414200	-1.20394000	0.05243500
1	-2.40790700	-0.01566800	0.13201200
1	0.00798900	0.08843500	-2.31400700
1	-0.05878700	-2.40155400	0.05760500
1	-0.00118500	-0.07049300	2.51245800
1	0.06278100	2.41429700	0.22102300
3	-1.73064300	-1.73395100	1.47099300

{Li2[BaHs]}* _conf0_MeCN E = -167.046347916 Ha

3	1.65533900	1.60571500	1.86247900
5	1.27638200	-0.01638400	0.05059900
1	2.45826800	0.00587500	0.10469700
5	0.00005300	1.28169400	0.09118000
5	-0.00057300	-0.02952000	1.17957700
5	0.00661600	0.04438000	-0.96553500
5	-1.27009300	0.03440100	0.04515300
5	0.00477900	-1.26326400	0.00416700
1	-2.45274300	0.00878100	0.08642300
1	-0.04202500	-2.44595200	0.00887000
1	0.00255100	-0.06691100	2.37431300
1	0.04599700	2.46087800	0.18167600
3	-1.69254300	-1.70812800	1.70990900

Li2[BaH7]_MeCN E = -193.318267060 Ha

5	8.29354000	19.09667500	4.10367700
1	9.08531100	19.01491700	5.00582100
5	6.94116400	20.01563300	4.18736400
1	6.65085100	20.66655300	5.15636000
5	6.13289700	19.86222200	2.77040000
1	5.09564600	20.37816000	2.44446000
5	6.98958900	18.84644400	1.80773700
1	6.69380400	18.51120600	0.70227200
5	8.32674200	18.37324100	2.63696000
1	9.15652500	17.62311100	2.18985400
5	7.91643100	20.13321100	2.66646100
1	8.52337700	21.06759800	2.28618000
5	6.75404900	18.34069400	3.52262600
1	6.15108600	17.41062900	3.97502900
3	5.02200900	21.20289300	4.21099900
3	10.14938200	17.83449900	3.85498300

{Li2[BaHs]}* _ap_MeCN E = -192.532570768 Ha

5	8.30598600	19.06265300	4.13858200
1	9.07944800	18.98953100	5.03902300

5	6.90553300	20.00446000	4.22763600
1	6.62676700	20.63796800	5.19443600
5	6.07713300	19.85349200	2.77022000
1	5.05750500	20.36375900	2.43239000
5	6.97158300	18.82026600	1.76820300
1	6.99433500	18.51219900	0.66402300
5	8.34836000	18.32732100	2.62479900
1	9.17181400	17.60086000	2.16801800
5	7.85744900	20.04838100	2.71546800
1	8.45154100	20.97380200	2.27299900
5	6.87971500	18.52611900	3.41618100
3	4.98991000	21.39726500	4.20736700
3	10.31423800	17.84898200	3.84598500

{Li2[BaHs]}* _eq_MeCN E = -192.506372318 Ha

5	8.18624100	19.14548700	4.02440300
5	6.94184800	20.06908300	4.22928600
1	6.60967400	20.73687500	5.15963100
5	6.14200900	19.89194300	2.78637900
1	5.11211700	20.41733600	2.47204900
5	7.04149700	18.84609000	1.86654700
1	6.88564100	18.41393800	0.77328500
5	8.42167200	18.36061500	2.72597700
1	9.12277200	17.60976600	2.13043200
5	7.87147100	20.21346400	2.62054800
1	8.49561200	21.12522800	2.19097600
5	6.65475200	18.36630000	3.52196000
1	6.07074400	17.44619000	3.98875200
3	4.82621000	21.19183700	4.25125500
3	10.41483100	17.52861700	3.71305600

Li2[BaHs]_MeCN E = -218.764986129 Ha

5	1.59856700	4.45509000	2.29475700
5	1.63108200	4.88111400	3.93756700
1	1.38502800	3.31716700	1.94241800
1	1.45998000	4.16521500	4.88638700
5	0.58395800	5.91266700	2.89874700
5	3.05290800	5.42427000	2.97566200
5	1.08067600	5.82851600	1.26748800
5	2.66086000	5.51600100	1.31673700
5	1.94202500	6.45117300	3.95103900
5	2.07794500	6.88451200	2.31553700
1	-0.56291300	6.13668400	3.15220900
1	4.18120100	5.19815900	3.30075800
1	0.32535400	5.98518600	0.35831300
1	3.47160100	5.36314500	0.45611600
1	2.05329500	7.16249100	4.91221400
1	2.31306600	8.02434400	1.98268300
3	1.26686900	2.63243500	3.70162100
3	2.33226000	6.89771000	3.75201900

{Li2[BaHs]}* _ap_MeCN E = -217.961262540 Ha

5	1.59220000	4.38555700	2.34192800
5	1.63802600	4.86379500	3.93770300
1	1.41393400	3.26805800	1.94918800
1	1.51894600	4.18895200	4.91633100
5	0.57890200	5.90021700	2.92377600
5	2.99276100	5.46478400	2.92737600
5	1.21326100	5.79273000	1.40747800
5	2.66962700	5.52166200	1.14319900
5	1.93950200	6.46725200	3.95040800
5	2.07351700	6.95308800	2.36168600
1	-0.57983200	6.11612900	3.07281100
1	4.15353000	5.22781800	3.05807300
1	3.61604800	5.34975300	0.46791000
1	2.07153700	7.12302000	4.94061400
1	2.31301300	8.06389900	1.98307600
3	1.05532700	2.58611500	3.80645800
3	2.26811100	8.79627200	3.85594400

{Li2[BaHs]}* _eq_MeCN E = -217.980272934 Ha

5	1.46343700	4.45674300	2.29081200
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5	1.60183100	4.86983200	3.95962200
1	1.24129400	3.32676400	1.96953900
1	1.46761900	4.09146900	4.85192100
5	0.55320300	5.90802700	2.92415500
5	2.84361800	5.47760800	2.95500900
5	1.13970300	5.81061000	1.27719000
5	2.80014500	5.49780900	1.39164800
5	1.90399700	6.47895900	2.16018000
5	1.92949200	6.93975600	2.30960600
1	-0.58664600	6.11986400	3.19218600
1	0.56735300	5.92560100	0.24601200
1	3.44313000	5.38469600	0.40937900
1	2.05761200	7.24082700	4.87498500
1	2.13306900	8.07894300	2.00883400
3	1.45249800	2.46221600	3.70592500
3	2.66120800	8.76841400	3.76289200

Li2[BaHs]_MeCN E = -244.241430062 Ha

3	1.70313000	-0.57344700	6.19060300
5	1.63958200	1.66317400	6.87164300
5	0.66739200	0.73113400	7.90758700
5	1.62108100	0.71239200	9.59012400
1	1.65725900	1.69000600	5.67308600
1	-0.00508100	-0.14953900	7.44213200
1	1.62866800	-0.16130100	10.40206500
5	2.62227400	0.77573000	7.93656100
5	2.58123900	2.54693900	7.97650200
5	0.62663600	2.50243900	7.94774000
5	0.17918900	1.57450400	9.29906900
5	3.03008100	1.63986000	9.34137600
1	3.34727400	-0.07329300	7.49113900
5	1.57985600	2.48818000	9.63057700
1	3.26552600	3.44765700	7.57058800
1	-0.08577400	3.37166000	7.52141000
1	-0.85496000	1.53672800	9.88188900
1	4.04752200	1.64933700	9.95416700
1	1.54811600	3.32291900	10.48195100
3	1.59427500	3.92432900	6.28406500

{Li2[BaHs]}* _ap_MeCN E = -243.425249665 Ha

3	1.62929900	-0.49512700	5.90247500
5	1.78647300	1.78067400	6.86078300
5	0.96188400	0.70294600	8.06002300
5	1.35475800	0.73405500	10.00052200
1	1.60498400	1.82784000	5.67684400
1	0.36194900	-0.24431900	7.63857200
1	1.11481600	-0.07666200	10.82550900
5	2.88065900	0.81606300	7.58657800
5	2.68690900	2.52864700	8.11930900
5	0.81489600	2.57049200	8.05197500
5	0.18741300	1.69298100	9.34804100
5	2.63865600	1.10211400	9.14179100
1	3.54207300	0.00019300	7.03061600
5	1.67580100	2.48875500	6.95381400
1	3.47358000	3.41354000	8.09497700
1	0.06128800	3.42326200	7.62911300
1	-0.95317200	1.71472700	9.66313700
1	1.96724000	3.35474300	10.40925400
3	0.55625600	3.63514600	5.78277400

{Li2[BaHs]}* _eq_MeCN E = -243.435127211 Ha

3	1.70449900	-0.68074900	6.20696200
5	1.64184300	1.72655500	6.88863200
5	0.66242800	0.75766000	7.91895200
5	1.62197400	0.65656400	9.59086100
1	1.66088300	1.76411000	5.69351600
1	-0.01031900	-0.12538000	7.47316800
1	1.62821500	-0.22407600	10.37560400
5	2.62863900	0.80084600	7.94925000
5	2.66102200	2.55932900	7.96595600
5	0.55380700	2.51221000	7.93160100

5	0.14839000	1.58376900	9.32019600
5	3.061		

1	3.708083000	7.139540000	5.076332000
1	-0.818172000	5.606961000	5.829588000
1	1.741379000	6.523402000	7.273720000
1	2.638442000	2.445021000	4.432576000
1	4.990721000	4.406608000	4.321257000
1	2.651641000	5.263148000	2.458919000
1	0.907145000	3.331426000	6.763995000
3	-0.084289000	4.857376000	7.825905000

{Li₂[B₁₁H₁₁]}⁻ MeCN E = -295.189448901 Ha

5	1.802065000	16.614537000	15.248607000
5	2.555538000	18.175385000	15.310389000
5	0.613800000	15.515608000	15.884957000
5	2.711467000	17.411863000	16.782770000
5	0.914014000	18.364852000	15.120722000
5	-0.159793000	16.919201000	15.455159000
5	1.659565000	15.954779000	17.093600000
5	1.659658000	18.842081000	16.655603000
5	-0.043176000	16.498868000	17.182794000
5	1.247296000	17.535303000	17.781972000
5	0.010748000	18.196139000	16.657947000
1	2.329506000	16.033966000	14.347878000
1	3.419488000	18.611144000	14.623944000
1	0.393489000	14.392388000	15.535370000
1	3.771281000	17.319703000	17.343029000
1	0.460802000	19.010933000	14.227392000
1	-1.115218000	16.955962000	14.720758000
1	2.252383000	15.136352000	17.725410000
1	1.901145000	19.935135000	17.091238000
1	-0.907109000	16.098498000	17.897370000
1	1.336022000	17.742326000	18.962371000
1	-0.894611000	18.920919000	16.927096000
3	2.995120000	18.907155000	18.623091000
3	-0.980034000	15.078852000	14.282136000

{Li₂[B₁₁H₁₀]}⁺ ap MeCN E = -294.378270974 Ha

5	1.667804000	16.750816000	15.460928000
5	2.573813000	18.177189000	15.303019000
5	0.583477000	15.504657000	15.887115000
5	2.762576000	17.425826000	16.784675000
5	0.930832000	18.395006000	15.095926000
5	-0.213326000	16.903536000	15.469781000
5	1.660193000	15.903466000	17.094447000
5	1.693238000	18.843245000	16.646167000
5	-0.040622000	16.482284000	17.193389000
5	1.283562000	17.519383000	17.778064000
5	0.022588000	18.192891000	16.653823000
1	3.438178000	18.501304000	14.566067000
1	0.430313000	14.405751000	15.454696000
1	3.812108000	17.289058000	17.323752000
1	0.457800000	18.995950000	14.195868000
1	-1.145113000	16.96184000	14.726970000
1	2.291093000	15.101383000	17.689163000
1	1.919605000	19.937035000	17.074565000
1	-0.890668000	16.098649000	17.924441000
1	1.390029000	17.685476000	18.959057000
1	-0.874394000	18.931115000	16.891642000
3	2.897871000	19.101450000	18.774639000
3	-1.047018000	15.026341000	14.185533000

{Li₂[B₁₁H₁₀]}⁻ eq1 MeCN E = -294.393271285 Ha

5	1.733790000	16.551092000	15.167372000
5	2.736060000	18.102323000	15.288215000
5	0.568586000	15.486357000	15.870451000
5	2.603984000	17.317639000	16.620082000
5	1.002663000	18.305110000	15.185728000
5	-0.144350000	16.946350000	15.491167000
5	1.728974000	15.907534000	16.995913000
5	1.732158000	18.826836000	16.677938000
5	0.022641000	16.477099000	17.212340000
5	1.350623000	17.484254000	17.786238000

5	0.086254000	18.190877000	16.713443000
1	2.245932000	16.038757000	14.226979000
1	3.436854000	18.578081000	14.474127000
1	0.287159000	14.381171000	15.528811000
1	0.724544000	17.838927000	14.222432000
1	-1.121182000	17.028614000	14.801966000
1	2.415719000	15.06014000	17.467791000
1	2.056416000	19.909602000	17.055815000
1	-0.813367000	16.081922000	17.953827000
1	1.545907000	17.635503000	18.954761000
1	-0.791800000	18.921257000	17.031187000
3	2.000813000	19.584919000	19.054847000
3	-1.246213000	15.097918000	14.3057143000

{Li₂[B₁₁H₁₀]}⁻ eq2 MeCN E = -294.390642608 Ha

5	1.832971000	16.646596000	15.271441000
5	2.564632000	18.208163000	15.321447000
5	0.477224000	15.505816000	15.834302000
5	2.700703000	17.415927000	16.794449000
5	0.896450000	18.338232000	15.139967000
5	0.005671000	16.968140000	15.596199000
5	1.610426000	16.014011000	17.046428000
5	1.667701000	18.875003000	16.671947000
5	-0.048451000	16.547759000	17.286723000
5	1.272827000	17.569009000	17.823171000
5	0.016522000	18.247221000	16.729645000
1	2.287263000	16.011255000	14.376806000
1	3.397627000	18.65696000	14.616314000
1	0.368825000	14.355721000	15.581682000
1	3.768133000	17.306601000	17.321387000
1	0.482114000	18.864551000	14.158218000
1	2.165803000	15.062791000	17.487150000
1	1.926281000	19.965051000	17.087791000
1	-0.927201000	16.141677000	17.964028000
1	1.389909000	17.775117000	18.994845000
1	-0.923994000	18.923714000	16.971767000
3	3.080455000	18.986239000	18.679844000
3	-0.963227000	14.830498000	14.005293000

Li₂[B₁₂H₁₂] MeCN E = -320.749960793 Ha

5	-0.782012000	-0.929927000	1.167789000
5	0.382290000	0.332676000	1.603693000
1	-1.361522000	-1.554000000	2.025086000
1	0.626555000	0.560701000	2.756942000
5	0.934413000	-1.168333000	0.835326000
1	1.571714000	-1.975210000	1.455689000
5	-0.274955000	-1.663559000	-0.361304000
1	-0.489951000	-2.808691000	-0.599599000
5	-1.164264000	0.775793000	0.878171000
1	-2.026498000	1.320171000	1.511218000
5	-1.567559000	-0.451445000	-0.338451000
1	-2.712218000	-0.745971000	-0.549410000
1	1.212049000	-0.842558000	-0.874051000
1	2.056669000	-1.414582000	-1.487108000
5	1.620080000	0.388005000	0.343784000
1	2.747313000	0.675023000	0.594110000
5	-0.894961000	1.108531000	-0.836156000
1	-1.551993000	1.908585000	-1.422861000
5	0.317144000	1.594560000	0.367580000
1	0.519431000	2.736545000	0.631789000
5	0.827483000	0.865183000	-1.165860000
1	1.398563000	1.498657000	-0.996759000
5	-0.340515000	-0.397668000	-1.602631000
1	-0.601057000	-0.651960000	-2.735601000
3	-3.187398000	-0.393638000	1.411198000
3	0.634614000	-1.448870000	3.180483000

{Li₂[B₁₂H₁₁]}⁻ conf1 MeCN E = -319.930565862 Ha

5	-0.793306000	-0.956581000	1.194336000
5	0.390016000	0.300507000	1.612008000
1	-1.362020000	-1.632391000	1.994447000

1	0.635956000	0.539069000	2.757756000
5	0.973150000	-1.196392000	0.852091000
1	1.572848000	-2.043514000	1.434804000
5	-0.219622000	-1.430076000	-0.324472000
5	-1.165672000	0.753920000	0.885783000
1	-2.012593000	1.308349000	1.522886000
5	-1.596720000	-0.447687000	-0.349254000
1	-2.711910000	-0.796864000	-0.580639000
5	1.257128000	-0.846917000	-0.900462000
1	2.062641000	-1.453572000	-1.517041000
5	1.638875000	0.370143000	0.346636000
1	2.761852000	0.652668000	0.597588000
5	-0.892306000	1.107671000	-0.836911000
1	-1.546716000	1.906978000	-1.417306000
5	0.321522000	1.554856000	0.372247000
1	0.525952000	2.690243000	0.644398000
5	0.842526000	0.863862000	-1.170152000
1	1.412065000	1.496319000	-1.995266000
5	-0.337195000	-0.382612000	-1.645104000
1	-0.598970000	-0.678950000	-2.758905000
3	-3.443311000	-0.152717000	1.298243000
3	0.669177000	-1.399605000	3.370444000

{Li₂[B₁₂H₁₁]}⁻ conf2 MeCN E = -319.93252087 Ha

5	-0.740923000	-0.989598000	1.067954000
5	0.294714000	0.162399000	1.752366000
1	0.531911000	0.311910000	2.908126000
5	0.900460000	-1.328487000	0.896889000
1	1.527932000	-2.135577000	1.506163000
5	-0.311747000	-1.800093000	-0.360214000
1	-0.518377000	-2.935720000	-0.613184000
5	-1.286622000	0.612725000	1.023666000
1	-2.171935000	1.082223000	1.663579000
5	-1.663350000	-0.598845000	-0.285765000
1	-2.794180000	-0.904136000	-0.492582000
5	1.161742000	-0.904236000	-0.809353000
1	2.023289000	-1.426316000	-1.433002000
5	1.521487000	0.282991000	0.472964000
1	2.645768000	0.581892000	0.750994000
5	-0.988440000	0.997649000	-0.684928000
1	-1.664706000	1.812281000	-1.241863000
5	0.199397000	1.469233000	0.550392000
1	0.3761444000	2.597571000	0.863580000
5	0.729966000	0.803054000	-1.009913000
1	1.288811000	1.487689000	-1.799687000
5	-0.400842000	-0.459118000	-1.530226000
1	-0.655386000	-0.662363000	-2.669376000
3	-3.402044000	1.299023000	-0.289018000
3	2.651868000	-0.484135000	2.530417000

Li₂[B₁₃H₁₃] MeCN E = -346.119377560 Ha

5	0.086542000	1.455103000	0.691524000
5	-0.025924000	-1.207540000	0.844128000
5	-1.352419000	0.204917000	1.232731000
5	1.389152000	0.086959000	1.171285000
1	0.142656000	2.556501000	1.146852000
1	-0.054095000	-2.260308000	1.403696000
5	0.031789000	0.193615000	2.043578000
5	-1.453458000	1.007216000	-0.340226000
5	-1.530778000	-0.746242000	-0.244619000
5	1.438263000	-0.857443000	-0.301235000
5	1.5195		

5	0.024318000	-0.077957000	2.032360000	5	-1.754436000	0.220372000	-0.906171000	1	0.132188000	2.427004000	1.487764000
5	-1.653178000	0.304517000	-0.791982000	5	-1.944909000	-1.160227000	0.130923000	1	-1.482322000	-2.300696000	2.194642000
5	-1.927164000	-1.134861000	0.156014000	5	0.869050000	-1.458905000	1.243428000	5	-0.581136000	-0.017963000	1.539885000
5	0.848370000	-1.456459000	1.183041000	5	1.517875000	1.091686000	-0.130774000	5	-1.103881000	0.960119000	-0.173457000
5	1.516475000	1.127904000	-0.158827000	5	-0.195243000	1.279414000	-0.748591000	5	-2.026862000	-1.874580000	-0.302571000
5	-0.078691000	1.353639000	-0.886035000	5	0.527886000	-1.363262000	-1.522836000	5	0.624614000	-1.602890000	1.033897000
5	0.539239000	-1.348042000	-1.458885000	5	1.159271000	0.251940000	-1.572552000	5	1.858164000	1.048214000	0.144019000
5	1.209740000	0.261596000	-1.604657000	5	-1.226132000	-1.420482000	-1.440815000	5	0.492408000	1.462664000	-0.880638000
5	-1.213240000	-1.352728000	-1.398690000	1	-0.153327000	0.121688000	3.238841000	5	0.836859000	-1.566661000	-1.050662000
1	-0.022691000	0.144822000	3.210661000	1	-2.179877000	1.028472000	1.442636000	5	1.537159000	0.150030000	-1.362269000
1	-2.257729000	0.862195000	1.641149000	1	2.546444000	0.308047000	2.006409000	5	-1.902367000	-0.343620000	-1.151041000
1	2.481637000	0.336349000	1.995918000	1	-2.742713000	0.770897000	-1.252418000	1	-0.934226000	0.286490000	2.644334000
1	-2.626013000	0.899538000	-1.130654000	1	-3.032545000	-1.527972000	0.423400000	1	-3.068205000	0.011881000	1.117261000
1	-3.046527000	-1.513330000	0.290289000	1	1.367659000	-2.365147000	1.814807000	1	1.788832000	0.104919000	2.561920000
1	1.464312000	-2.305407000	1.744227000	1	2.305174000	1.968222000	-0.254926000	1	-1.812572000	1.928715000	-0.207940000
1	2.308639000	2.011187000	-0.220158000	1	-0.447275000	2.381434000	-1.109822000	1	-2.980927000	-2.564503000	-0.416213000
1	-0.295230000	2.453575000	-1.284009000	1	1.005235000	-0.134809000	-2.301085000	1	1.223806000	-2.353318000	1.734262000
1	1.001882000	-2.139719000	-2.235397000	1	1.901028000	0.542536000	-2.467174000	1	2.847140000	1.679512000	0.259705000
1	1.963105000	0.481873000	-2.512466000	1	-1.804580000	-2.127750000	-2.194474000	1	0.457663000	2.468970000	-1.501934000
1	-1.798913000	-2.031167000	-2.179807000	3	1.428336000	1.763219000	3.251571000	1	1.554910000	-2.287779000	-1.675540000
3	1.279730000	1.701160000	3.104549000	3	1.032104000	-0.575719000	-3.906888000	1	2.290410000	0.169402000	-2.272082000
3	0.979700000	-0.741117000	-3.798206000	5	-0.490522000	0.022018000	-2.042599000	1	-2.758195000	0.051368000	-1.867632000
5	-0.455661000	0.068581000	-2.025704000	1	-0.710671000	0.354212000	-3.169499000	3	-2.203888000	1.935167000	1.893458000
1	-0.714912000	0.346953000	-3.163031000	5	1.784680000	-0.720337000	-0.253104000	3	0.482115000	-1.430419000	-3.809414000
5	1.805188000	-0.686050000	-0.257589000	1	2.846316000	-1.225422000	-0.404414000	5	-0.233425000	0.026213000	-1.762213000
1	2.883085000	-1.166458000	-0.406101000	5	-0.351297000	-2.142871000	-0.073971000	1	-0.309748000	0.316674000	-2.924260000
5	-0.397099000	-2.130206000	-0.047412000	1	-0.315466000	-3.322389000	0.006111000	5	1.692088000	-0.629060000	0.104361000
1	-0.385859000	-3.319778000	-0.091055000					5	-0.418356000	-2.534877000	-0.140193000
{Li₂[B₁₆H₁₆]}*_{ap}_MeCN E = -421.698936244 Ha				Li₂[B₁₇H₁₇]_{MeCN} E = -447.973689147 Ha				{Li₂[B₁₇H₁₆]}*_eq_MeCN E = -447.185779009 Ha			
5	0.174033000	1.259396000	0.789445000	5	0.303504000	1.408673000	0.835999000	5	0.320973000	1.426232000	0.837105000
5	-0.940945000	-1.403404000	1.572884000	5	-1.162784000	-1.708587000	1.207310000	5	-1.141876000	-1.723894000	1.233518000
5	-1.420909000	0.271823000	1.041394000	5	-2.089555000	-0.369199000	0.586993000	5	-2.115315000	-0.386762000	0.581347000
5	1.567413000	0.158790000	1.235131000	5	1.235538000	0.072922000	1.456437000	5	1.235624000	0.046056000	1.484202000
1	0.101370000	2.365832000	1.238884000	1	0.132251000	2.407854000	1.469850000	1	0.166349000	2.407849000	1.491990000
1	-1.317598000	-2.032556000	2.502544000	1	-1.486827000	-2.290517000	2.190182000	1	-1.373211000	-2.231000000	2.274226000
5	0.015733000	-0.027388000	1.971143000	5	-0.570348000	-0.027335000	1.519282000	5	-0.605343000	0.020668000	1.473184000
5	-1.577031000	0.231109000	-0.817351000	5	-1.130851000	0.964265000	-0.178707000	5	-1.124486000	0.950026000	-0.167191000
5	-1.984993000	-1.168523000	0.202199000	5	-2.045711000	-1.870601000	-0.295420000	5	-2.036686000	-1.913461000	-0.270978000
5	0.804980000	-1.461212000	1.118994000	5	0.638610000	-1.581992000	0.997560000	5	0.486083000	-1.346674000	0.777084000
5	1.598796000	1.034026000	-0.258922000	5	1.835818000	1.012907000	0.107587000	5	1.866562000	0.992481000	0.140214000
5	0.024187000	1.196711000	-1.050622000	5	0.463998000	1.442934000	-0.895367000	5	0.495309000	1.441293000	-0.879388000
5	0.475869000	-1.354318000	-0.956987000	5	0.820555000	-1.544150000	-1.030966000	5	0.794835000	-1.499530000	-1.074483000
5	1.310561000	0.015365000	-1.631765000	5	1.490503000	0.112417000	-1.343041000	5	1.516269000	0.128436000	-1.340969000
5	-1.216556000	-1.530141000	-1.315817000	5	-1.937424000	-0.341361000	-1.145154000	5	-1.946460000	-0.375788000	-1.135995000
1	-0.006579000	0.245030000	3.136369000	5	-0.919087000	0.288544000	2.628254000	1	-0.924171000	0.288869000	2.590214000
1	-2.270312000	0.906466000	1.572847000	1	-3.077113000	0.024105000	1.134973000	1	-3.092709000	-0.019105000	1.151312000
1	2.446031000	0.365214000	2.016008000	1	1.748795000	0.113492000	2.526204000	1	1.642985000	0.014161000	2.591798000
1	-2.519530000	0.809083000	-1.246657000	1	-1.847972000	1.931321000	-0.197251000	1	-1.837227000	1.915632000	-0.201722000
1	-3.124982000	-1.473476000	0.305694000	1	-2.995486000	-2.573368000	-0.394519000	1	-2.979143000	-2.619626000	-0.367035000
1	1.413779000	-2.323550000	1.656315000	1	1.143855000	-2.366606000	1.739541000	1	2.812232000	1.693555000	0.241281000
1	2.380229000	1.916258000	-0.368829000	1	2.782892000	-1.719895000	0.202155000	1	0.470125000	2.450589000	-1.496050000
1	-0.114576000	2.250539000	-1.600741000	1	0.423627000	2.452189000	-1.518644000	1	1.438938000	-2.275714000	-1.710323000
1	1.973478000	0.061778000	-2.617461000	1	1.453595000	-2.298846000	-1.724991000	1	2.237957000	0.155347000	-2.286844000
1	-1.700845000	-2.211684000	-2.150032000	1	2.192895000	0.160728000	-2.309997000	1	-2.816471000	0.005110000	-1.841361000
3	1.230168000	1.793184000	3.102993000	1	-2.803343000	0.056085000	-1.852783000	3	-2.131597000	2.081758000	1.869912000
3	0.558416000	1.634514000	-3.508843000	3	-2.062893000	1.907538000	1.906298000	3	0.826326000	-1.182895000	-3.663572000
5	-0.387979000	-0.176680000	-2.021375000	3	0.921495000	-1.292488000	-3.476452000	5	-0.258508000	0.009659000	-1.744652000
1	-0.634191000	-0.061662000	-3.180222000	5	-0.271212000	0.026988000	-1.756534000	1	-0.358096000	0.307471000	-2.903771000
5	1.949535000	-0.728139000	-0.201842000	1	-0.361254000	0.312980000	-2.922454000	5	1.981627000	-0.764155000	0.124514000
1	2.989010000	-1.284681000	-0.275520000	5	1.973249000	-0.731793000	0.102963000	1	2.962374000	-1.418228000	0.188106000
5	-0.569202000	-2.275858000	0.114873000	1	3.024199000	-1.277644000	0.186610000	5	-0.395557000	-2.534051000	-0.126004000
1	-0.532448000	-3.456704000	0.161173000	5	-0.424814000	-2.513219000	-0.146458000	1	-0.054326000	-3.664140000	-0.129259000
				1	-0.210861000	-3.681075000	-0.149576000	5	-0.918491000	-1.683870000	-1.597625000
				5	-0.900942000	-1.664525000	-1.592604000	1	-1.015539000	-2.268149000	-2.629907000
				1	-1.013694000	-2.220988000	-2.644862000				
{Li₂[B₁₆H₁₆]}*_eq_MeCN E = -421.696171733 Ha				{Li₂[B₁₇H₁₆]}*_ap_MeCN E = -447.151782972 Ha							
5	0.284842000	1.324702000	1.040853000	5	0.308914000	1.431959000	0.858486000	5	-0.918491000	-1.683870000	-1.597625000
5	-0.778533000	-1.209258000	1.262126000	5	-1.162113000	-1.723707000	1.211513000	1	-1.015539000	-2.268149000	-2.629907000
5	-1.324709000	0.436552000	0.878847000	5	-2.072956000	-0.373092000	0.581983000				
5	1.597445000	0.121729000	1.306472000	5	1.226342000	0.102633000	1.526065000				
1	0.236918000	2.382857000	1.592627000								
5	0.039957000	-0.050537000	2.077355000								