Flattening the $B_6H_6^{2-}$ Octahedron. Ab Initio Prediction of New Family of Planar All-Boron Aromatic Molecules.

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Supporting Information

Figure 1S. Discovered aromatic structures $B_xH_yLi_z$ and corresponding uncharged and slightly charged Boron Hydrides.

() – B3LYP/6-311++G** level of theory

[] – MP2/6-311++G** level of theory

{ } – CASSCF(8,8)/6-311++G** level of theory

Figure 2S. Molecular orbitals picture of $\text{B}_6\text{H}_6\text{Li}_6$ and C_6H_6 (RHF/6-311++G** level of theory).

Figure 3S. Alternative structures of $B_6H_6Li_6$ species (B3LYP/6-311++G** level of theory).

Table 1S. Molecular Properties of structure A - B₆H₆Li₆ (Fig.1)

Geometry:

Center Number	Atomic Simbol	Coordinates								
		B3LYP/6-311++G**			CASSCF(8,8)/6-311++G**			MP2/6-311++G**		
		X	Y	Z	X	Y	Z	X	Y	Z
1	B	1.6824	0.0000	0.0000	1.7021	0.0000	0.0000	1.6959	0.0000	0.0000
2	Li	0.0000	0.0000	1.5019	0.0000	0.0000	1.5434	0.0000	0.0000	1.5235
3	Li	0.0000	0.0000	-1.5019	0.0000	0.0000	-1.5434	0.0000	0.0000	-1.5235
4	B	-1.6824	0.0000	0.0000	-1.7021	0.0000	0.0000	-1.6959	0.0000	0.0000
5	B	0.8278	1.4568	0.0000	0.8367	1.4741	0.0000	0.8331	1.4639	0.0000
6	B	0.8278	-1.4568	0.0000	0.8367	-1.4741	0.0000	0.8331	-1.4639	0.0000
7	B	-0.8278	-1.4568	0.0000	-0.8367	-1.4741	0.0000	-0.8331	-1.4639	0.0000
8	B	-0.8278	1.4568	0.0000	-0.8367	1.4741	0.0000	-0.8331	1.4639	0.0000
9	H	2.9792	0.0000	0.0000	3.0076	0.0000	0.0000	2.9887	0.0000	0.0000
10	H	-2.9792	0.0000	0.0000	-3.0076	0.0000	0.0000	-2.9887	0.0000	0.0000
11	H	1.3588	2.5850	0.0000	1.3783	2.6040	0.0000	1.3543	2.5981	0.0000
12	H	1.3588	-2.5850	0.0000	1.3783	-2.6040	0.0000	1.3543	-2.5981	0.0000
13	H	-1.3588	-2.5850	0.0000	-1.3783	-2.6040	0.0000	-1.3543	-2.5981	0.0000
14	H	-1.3588	2.5850	0.0000	-1.3783	2.6040	0.0000	-1.3543	2.5981	0.0000
15	Li	2.8387	1.7469	0.0000	2.8663	1.7686	0.0000	2.8736	1.7784	0.0000
16	Li	2.8387	-1.7469	0.0000	2.8663	-1.7686	0.0000	2.8736	-1.7784	0.0000
17	Li	-2.8387	-1.7469	0.0000	-2.8663	-1.7686	0.0000	-2.8736	-1.7784	0.0000
18	Li	-2.8387	1.7469	0.0000	-2.8663	1.7686	0.0000	-2.8736	1.7784	0.0000

Other Properties:

	B3LYP/6-311++G**		CASSCF(8,8)/ 6-311++G**		MP2/ 6-311++G**
E _{total} , a.u.	-198.077083**		-196.4171543		-196.3185709
NImag	0		0		*
ZPE, kcal/mol	55.73372		58.00506		*
Frequencies	ν_1 (a _g)2190.7	ν_{25} (a _u)756.6	ν_1 (a _g)2216.4	ν_{25} (a _u)854.7	*
	ν_2 (a _g)1834.6	ν_{26} (a _u)374.1	ν_2 (a _g)1836.9	ν_{26} (a _u)357.0	*
	ν_3 (a _g)1234.1	ν_{27} (a _u)53.9	ν_3 (a _g)1331.7	ν_{27} (a _u)69.9	*
	ν_4 (a _g)1080.1	ν_{28} (b _{1u})706.9	ν_4 (a _g)1152.2	ν_{28} (b _{1u})777.7	*
	ν_5 (a _g)732.1	ν_{29} (b _{1u})554.9	ν_5 (a _g)747.8	ν_{29} (b _{1u})596.4	*
	ν_6 (a _g)518.2	ν_{30} (b _{1u})432.4	ν_6 (a _g)532.4	ν_{30} (b _{1u})423.8	*
	ν_7 (a _g)463.3	ν_{31} (b _{1u})343.3	ν_7 (a _g)470.4	ν_{31} (b _{1u})370.3	*
	ν_8 (a _g)413.2	ν_{32} (b _{1u})61.1	ν_8 (a _g)411.9	ν_{32} (b _{1u})65.1	*
	ν_9 (a _g)342.4	ν_{33} (b _{2u})2173.7	ν_9 (a _g)356.6	ν_{33} (b _{2u})2197.4	*
	ν_{10} (b _{1g})2149.5	ν_{34} (b _{2u})1394.5	ν_{10} (b _{1g})2171.0	ν_{34} (b _{2u})1470.0	*
	ν_{11} (b _{1g})1378.2	ν_{35} (b _{2u})1199.1	ν_{11} (b _{1g})1452.0	ν_{35} (b _{2u})1265.5	*
	ν_{12} (b _{1g})1251.8	ν_{36} (b _{2u})999.9	ν_{12} (b _{1g})1343.2	ν_{36} (b _{2u})1029.1	*
	ν_{13} (b _{1g})991.1	ν_{37} (b _{2u})902.3	ν_{13} (b _{1g})1023.4	ν_{37} (b _{2u})914.5	*
	ν_{14} (b _{1g})646.7	ν_{38} (b _{2u})521.4	ν_{14} (b _{1g})656.8	ν_{38} (b _{2u})564.5	*
	ν_{15} (b _{1g})510.1	ν_{39} (b _{2u})416.0	ν_{15} (b _{1g})528.3	ν_{39} (b _{2u})517.4	*
	ν_{16} (b _{1g})384.9	ν_{40} (b _{2u})316.7	ν_{16} (b _{1g})404.1	ν_{40} (b _{2u})328.8	*
	ν_{17} (b _{2g})748.2	ν_{41} (b _{3u})2158.6	ν_{17} (b _{2g})820.2	ν_{41} (b _{3u})2180.5	*
	ν_{18} (b _{2g})620.3	ν_{42} (b _{3u})1825.3	ν_{18} (b _{2g})678.7	ν_{42} (b _{3u})1831.3	*
	ν_{19} (b _{2g})517.0	ν_{43} (b _{3u})1267.6	ν_{19} (b _{2g})547.5	ν_{43} (b _{3u})1359.3	*
	ν_{20} (b _{2g})428.5	ν_{44} (b _{3u})825.1	ν_{20} (b _{2g})433.2	ν_{44} (b _{3u})846.8	*
	ν_{21} (b _{2g})62.8	ν_{45} (b _{3u})722.7	ν_{21} (b _{2g})79.9	ν_{45} (b _{3u})760.5	*
	ν_{22} (b _{3g})612.0	ν_{46} (b _{3u})609.1	ν_{22} (b _{3g})666.5	ν_{46} (b _{3u})607.2	*
	ν_{23} (b _{3g})435.3	ν_{47} (b _{3u})395.5	ν_{23} (b _{3g})433.6	ν_{47} (b _{3u})407.6	*
	ν_{24} (b _{3g})82.3	ν_{48} (b _{3u})348.0	ν_{24} (b _{3g})85.9	ν_{48} (b _{3u})399.3	*

*- frequencies were not calculated at this level of theory

** - E_{total} (CCSD(T)/6-311++G**) = -197.1957259

Table 2S. Molecular properties of low-lying isomers of $B_6H_6Li_6$ (Fig. 2) at the B3LYP/6-311++G** level of theory:

Table 2S.1. Isomer B - C_1 (1A)

Geometry:

Center Number	Atomic Simbol	Coordinates		
		X	Y	Z
1	Li	4.5084	-0.7294	-0.9577
2	H	0.4801	-0.2214	-1.7382
3	B	-0.084266	-0.0263	-0.6683
4	B	-0.7765	1.5223	-0.0955
5	B	-1.8220	0.2634	-0.3829
6	B	-1.1217	-1.1577	0.2532
7	B	0.3408	-0.7433	0.9353
8	B	0.5504	0.9113	0.7412
9	H	-0.7325	2.5580	-0.7487
10	H	-2.7132	0.2794	-1.2344
11	H	-1.4319	-2.3063	-0.7002
12	H	1.2365	-1.5679	1.1254
13	H	1.6369	1.5049	0.7446
14	Li	1.0829	1.9458	-1.0684
15	Li	-2.8927	-1.4524	-0.7676
16	Li	1.5732	-1.4857	-0.8506
17	Li	2.4303	-1.009	1.2043
18	LI	-1.3387	0.4573	1.7755

Other Properties:

E _{total} , a.u.	-198.0600761		
NImag	0		
ZPE, kcal/mol	55.91281		
Frequencies	v ₁ 2346.8	v ₁₇ 883.7	v ₃₃ 475.0
	v ₂ 2318.8	v ₁₈ 867.6	v ₃₄ 431.9
	v ₃ 2289.1	v ₁₉ 837.4	v ₃₅ 423.9
	v ₄ 2281.3	v ₈₀ 826.0	v ₃₆ 383.9
	v ₅ 2260.5	v ₂₁ 812.3	v ₃₇ 374.7
	v ₆ 2228.6	v ₂₂ 759.1	v ₃₈ 351.6
	v ₇ 1180.6	v ₂₃ 713.5	v ₃₉ 339.2
	v ₈ 1110.7	v ₂₄ 674.8	v ₄₀ 283.4
	v ₉ 1099.2	v ₂₅ 645.5	v ₄₁ 273.2
	v ₁₀ 1030.5	v ₂₆ 641.8	v ₄₂ 228.3
	v ₁₁ 1021.0	v ₂₇ 616.8	v ₄₃ 201.4
	v ₁₂ 996.5	v ₂₈ 600.9	v ₄₄ 163.7
	v ₁₃ 934.2	v ₂₉ 546.8	v ₄₅ 136.1
	v ₁₄ 915.0	v ₃₀ 541.5	v ₄₆ 116.4
	v ₁₅ 907.9	v ₃₁ 519.4	v ₄₇ 73.9
	v ₁₆ 889.0	v ₃₂ 507.0	v ₄₈ 51.8

Table 2S.2. Isomer E – C_s (¹A').

Geometry:

Center Number	Atomic Simbol	Coordinates		
		X	Y	Z
1	B	0.3030	0.3322	1.8704
2	B	0.0501	0.1450	0.7039
3	B	-0.7617	-1.3259	-0.0229
4	B	-1.6023	0.1665	-0.0799
5	B	-0.4968	1.3588	-0.5898
6	B	0.9787	0.6084	-0.8297
7	H	0.8111	-1.0506	0.5807
8	H	-1.1424	-2.3314	-0.5013
9	H	-2.6573	0.3887	0.5795
10	H	-0.6085	2.5714	-0.4030
11	H	2.0254	1.2462	-0.8745
12	H	1.7079	-1.8456	-0.2390
13	Li	-0.6520	-0.3387	-2.1179
14	Li	1.8381	-1.2349	1.8223
15	Li	-2.8403	-1.5683	0.4675
16	Li	-1.8232	2.1301	1.2089
17	Li	2.2103	1.5034	0.9388
18	Li	3.0925	-0.4491	-0.6246

Other Properties:

E _{total} , a.u.	-198.0159465		
NImag	0		
ZPE, kcal/mol	54.62200		
Frequencies	ν_1 (a') 2154.3	ν_{17} (a') 438.4	ν_{33} (a'') 1271.8
	ν_2 (a') 1956.7	ν_{18} (a') 410.3	ν_{34} (a'') 1037.7
	ν_3 (a') 1835.8	ν_{19} (a') 409.1	ν_{35} (a'') 860.1
	ν_4 (a') 1398.9	ν_{80} (a') 401.5	ν_{36} (a'') 758.1
	ν_5 (a') 1271.3	ν_{21} (a') 371.4	ν_{37} (a'') 742.1
	ν_6 (a') 1216.9	ν_{22} (a') 366.6	ν_{38} (a'') 665.6
	ν_7 (a') 1091.6	ν_{23} (a') 326.1	ν_{39} (a'') 618.6
	ν_8 (a') 1023.3	ν_{24} (a') 235.0	ν_{40} (a'') 609.7
	ν_9 (a') 916.9	ν_{25} (a') 151.7	ν_{41} (a'') 572.6
	ν_{10} (a') 748.1	ν_{26} (a') 88.9	ν_{42} (a'') 540.1
	ν_{11} (a') 703.2	ν_{27} (a') 66.8	ν_{43} (a'') 492.1
	ν_{12} (a') 639.5	ν_{28} (a'') 2124.0	ν_{44} (a'') 380.6
	ν_{13} (a') 578.4	ν_{29} (a'') 1913.4	ν_{45} (a'') 333.8
	ν_{14} (a') 533.3	ν_{30} (a'') 1834.1	ν_{46} (a'') 245.4
	ν_{15} (a') 509.6	ν_{31} (a'') 1382.1	ν_{47} (a'') 117.0
	ν_{16} (a') 474.7	ν_{32} (a'') 1322.3	ν_{48} (a'') 68.8

Table 2S.3. Isomer F – D_{3d} ($^1A_{1g}$).

Geometry:

Center Number	Atomic Simbol	Coordinates		
		X	Y	Z
1	Li	-2.4671	1.4244	1.1682
2	Li	2.4671	1.4244	1.1682
3	Li	0.0000	-2.8488	1.1682
4	B	0.0000	0.9767	0.9037
5	B	0.8458	-0.4883	0.9037
6	B	-0.8458	-0.4883	0.9037
7	B	-0.8458	0.4883	-0.9037
8	B	0.8458	0.4883	-0.9037
9	B	0.0000	-0.9767	-0.9037
10	Li	0.0000	2.8488	-1.1682
11	Li	2.4671	-1.4244	-1.1682
12	Li	-2.4671	-1.4244	-1.1682
13	H	0.0000	2.1710	0.9037
14	H	1.8801	-1.0855	0.9037
15	H	-1.8801	-1.0855	0.9037
16	H	-1.8801	1.0855	-0.9037
17	H	1.8801	1.0855	-0.9037
18	H	0.0000	-2.1710	-0.9037

Other Properties:

E _{total} , a.u.	-197.9740785	
NImag	6	
ZPE, kcal/mol	52.45483	
Frequencies	ν_1 (a _{1g}) 2548.2	ν_{17} (e _g) 2515.2
	ν_2 (a _{1g}) 990.3	ν_{18} (e _g) 875.5
	ν_3 (a _{1g}) 790.9	ν_{19} (e _g) 825.0
	ν_4 (a _{1g}) 698.7	ν_{20} (e _g) 765.3
	ν_5 (a _{1g}) 346.8	ν_{21} (e _g) 683.4
	ν_6 (a _{1g}) 205.2	ν_{22} (e _g) 258.8
	ν_7 (a _{2g}) 884.8	ν_{23} (e _g) 130.7
	ν_8 (a _{1u}) 879.3	ν_{24} (e _g) 87.1i
	ν_9 (a _{1u}) 478.2	ν_{25} (e _u) 2524.5
	ν_{10} (a _{1u}) 65.8i	ν_{26} (e _u) 1074.7
	ν_{11} (a _{2u}) 2533.9	ν_{27} (e _u) 866.2
	ν_{12} (a _{2u}) 1028.3	ν_{28} (e _u) 732.5
	ν_{13} (a _{2u}) 718.9	ν_{29} (e _u) 436.1
	ν_{14} (a _{2u}) 342.8	ν_{30} (e _u) 258.5
	ν_{15} (a _{2u}) 210.5	ν_{31} (e _u) 71.5
	ν_{16} (a _{2u}) 91.5i	ν_{32} (e _u) 86.4i

Table 3S. Molecular Properties of structure B – B₅H₅Li₆ (Fig.1) at the B3LYP/6-311++G** level of theory.

Geometry:

Center Number	Atomic Simbol	Coordinates		
		X	Y	Z
1	B	0.0000	1.2764	0.0000
2	Li	1.6499	-0.1898	0.0000
3	Li	-1.7252	-0.1279	0.0000
4	B	-0.0318	0.2592	1.3737
5	B	-0.0318	0.2592	-1.3737
6	B	-0.0718	-1.3514	0.8307
7	B	-0.0718	-1.3514	-0.8307
8	B	-0.0741	2.5399	0.0000
9	H	-0.0460	0.6633	2.5799
10	H	-0.0460	0.6633	-2.5799
11	H	-0.0762	-2.3696	1.5434
12	H	-0.0762	-2.3696	-1.5434
13	H	0.3052	2.2531	1.7659
14	H	0.3052	2.2531	-1.7659
15	Li	-0.0415	-1.1922	2.8337
16	Li	-0.0415	-1.1922	-2.8337

Other Properties:

E _{total} , a.u.	-172.5752628	
NImag	0	
ZPE, kcal/mol	46.64395	
Frequencies	ν_1 (a') 2219.2	ν_{22} (a') 433.8
	ν_2 (a') 2055.4	ν_{23} (a') 430.2
	ν_3 (a') 1999.2	ν_{24} (a') 377.3
	ν_4 (a') 1237.8	ν_{25} (a') 362.5
	ν_5 (a') 1234.0	ν_{26} (a') 314.6
	ν_6 (a') 1120.0	ν_{27} (a') 311.3
	ν_7 (a') 981.1	ν_{28} (a') 305.5
	ν_8 (a') 860.9	ν_{29} (a') 108.4
	ν_9 (a') 839.9	ν_{30} (a') 107.3
	ν_{10} (a') 806.5	ν_{31} (a') 93.2
	ν_{11} (a') 644.0	ν_{32} (a') 88.7
	ν_{12} (a') 638.2	ν_{33} (a') 2196.2
	ν_{13} (a') 621.7	ν_{34} (a') 2000.1
	ν_{14} (a') 620.2	ν_{35} (a') 1183.9
	ν_{15} (a') 544.9	ν_{36} (a') 1161.5
	ν_{16} (a') 543.7	ν_{37} (a') 917.6
	ν_{17} (a') 524.4	ν_{38} (a') 711.9
	ν_{18} (a') 489.5	ν_{39} (a') 675.2
	ν_{19} (a') 477.9	ν_{40} (a') 552.1
	ν_{80} (a') 467.6	ν_{41} (a') 475.4
	ν_{21} (a') 453.8	ν_{42} (a') 441.0

Table 4S. Molecular Properties of structure C – B₇H₇Li₆ (C_s, ¹A') (Fig.1) at the B3LYP/6-311++G** level of theory.

Geometry:

Center Number	Atomic Simbol	Coordinates		
		X	Y	Z
1	B	0.0012	-2.0833	-0.2621
2	B	-1.5115	-1.3501	-0.1532
3	B	-1.8801	0.2822	0.0395
4	B	-0.8321	1.6010	0.1792
5	B	0.8301	1.6011	0.1805
6	B	1.8798	0.2836	0.0414
7	B	1.5134	-1.3493	-0.1512
8	H	0.0016	-3.2774	-0.4561
9	H	-2.4470	-2.1899	-0.2180
10	H	-3.1717	0.5847	0.0844
11	H	-1.3014	2.7592	0.3067
12	H	1.2993	2.7595	0.3085
13	H	3.1706	0.5891	0.0871
14	H	2.4495	-2.1887	-0.2141
15	Li	-0.0004	-0.2985	1.4024
16	Li	0.0010	0.0219	-1.4355
17	Li	-3.5210	-1.1078	0.6230
18	Li	-2.7889	2.2490	-0.4813
19	Li	3.5238	-1.1029	0.6223
20	Li	2.7838	2.2506	-0.4875

Other Properties:

E _{total} , a.u.	-223.5624361		
NImag	0		
ZPE, kcal/mol	66.19192		
Frequencies	v ₁ 2549.1	v ₁₉ 916.4	v ₃₇ 416.8
	v ₂ 2183.3	v ₈₀ 894.0	v ₃₈ 414.2
	v ₃ 2140.1	v ₂₁ 890.2	v ₃₉ 404.4
	v ₄ 2139.1	v ₂₂ 860.8	v ₄₀ 400.0
	v ₅ 2126.5	v ₂₃ 823.8	v ₄₁ 388.8
	v ₆ 1675.6	v ₂₄ 767.0	v ₄₂ 382.7
	v ₇ 1669.1	v ₂₅ 732.0	v ₄₃ 373.7
	v ₈ 1472.7	v ₂₆ 713.3	v ₄₄ 365.6
	v ₉ 1463.5	v ₂₇ 689.9	v ₄₅ 346.5
	v ₁₀ 1341.1	v ₂₈ 679.5	v ₄₆ 319.1
	v ₁₁ 1337.3	v ₂₉ 665.8	v ₄₇ 318.5
	v ₁₂ 1315.0	v ₃₀ 587.7	v ₄₈ 314.2
	v ₁₃ 1280.8	v ₃₁ 568.0	v ₄₉ 244.1
	v ₁₄ 1151.44	v ₃₂ 534.2	v ₅₀ 238.6
	v ₁₅ 1123.9	v ₃₃ 487.2	v ₅₁ 106.2
	v ₁₆ 1101.3	v ₃₄ 485.5	v ₅₂ 94.6
	v ₁₇ 1034.5	v ₃₅ 474.1	v ₅₃ 77.2
	v ₁₈ 1000.1	v ₃₆ 451.9	v ₅₄ 75.0

Table 5S. Molecular Properties of structure D – B₁₀H₈Li₁₀ (C_{2h}, ¹A_g) (Fig.1) at the B3LYP/6-311++G** level of theory.

Geometry:

Center Number	Atomic Simbol	Coordinates		
		X	Y	Z
1	B	0.0000	0.8904	0.0000
2	B	0.0000	-0.8904	0.0000
3	B	0.0194	1.6650	1.5603
4	B	-0.0194	-1.6650	1.5603
5	B	-0.0194	-1.6650	-1.5603
6	B	0.0194	1.6650	-1.5603
7	B	0.0170	0.8380	-3.0053
8	B	0.0170	0.8380	3.0053
9	B	-0.0170	-0.8380	3.0053
10	B	-0.0170	-0.8380	-3.0053
11	H	0.1033	2.9582	-1.5477
12	H	0.1033	2.9582	1.5477
13	H	-0.1033	-2.9582	1.5477
14	H	-0.1033	-2.9582	-1.5477
15	H	0.0617	1.3718	-4.1300
16	H	0.0617	1.3718	4.1300
17	H	-0.0617	-1.3718	4.1300
18	H	-0.0617	-1.3718	-4.1300
19	Li	-0.7544	2.8514	0.0000
20	Li	0.7544	-2.8514	0.0000
21	Li	1.4429	-0.0206	-1.5289
22	Li	1.4429	-0.0206	1.5289
23	Li	-1.4429	0.0206	1.5289
24	Li	-1.4429	0.0206	-1.5289
25	Li	0.0084	2.8501	-3.2730
26	Li	0.0084	2.8501	3.2730
27	Li	-0.0084	-2.8501	3.2730
28	Li	-0.0084	-2.8501	-3.2730

Other Properties:

E _{total} , a.u.	-328.956967		
NImag	0		
ZPE, kcal/mol			
Frequencies	$\nu_1(a_g)$ 2191.7	$\nu_{27}(b_g)$ 837.4	$\nu_{53}(a_u)$ 447.5
	$\nu_2(a_g)$ 1856.8	$\nu_{28}(b_g)$ 747.0	$\nu_{54}(a_u)$ 389.7
	$\nu_3(a_g)$ 1361.9	$\nu_{29}(b_g)$ 721.3	$\nu_{55}(a_u)$ 379.3
	$\nu_4(a_g)$ 1197.5	$\nu_{30}(b_g)$ 624.6	$\nu_{56}(a_u)$ 322.9
	$\nu_5(a_g)$ 1050.4	$\nu_{31}(b_g)$ 597.2	$\nu_{57}(a_u)$ 166.6
	$\nu_6(a_g)$ 896.6	$\nu_{32}(b_g)$ 537.7	$\nu_{58}(a_u)$ 45.6
	$\nu_7(a_g)$ 827.5	$\nu_{33}(b_g)$ 463.1	$\nu_{59}(b_u)$ 2163.1
	$\nu_8(a_g)$ 767.6	$\nu_{34}(b_g)$ 439.8	$\nu_{60}(b_u)$ 1840.6
	$\nu_9(a_g)$ 695.2	$\nu_{35}(b_g)$ 397.4	$\nu_{61}(b_u)$ 1350.3
	$\nu_{10}(a_g)$ 661.4	$\nu_{36}(b_g)$ 373.1	$\nu_{62}(b_u)$ 1251.3
	$\nu_{11}(a_g)$ 603.8	$\nu_{37}(b_g)$ 296.2	$\nu_{63}(b_u)$ 975.6
	$\nu_{12}(a_g)$ 509.4	$\nu_{38}(b_g)$ 283.3	$\nu_{64}(b_u)$ 829.6
	$\nu_{13}(a_g)$ 474.7	$\nu_{39}(b_g)$ 89.4	$\nu_{65}(b_u)$ 739.5
	$\nu_{14}(a_g)$ 465.5	$\nu_{40}(a_u)$ 2185.6	$\nu_{66}(b_u)$ 642.1
	$\nu_{15}(a_g)$ 421.2	$\nu_{41}(a_u)$ 1814.5	$\nu_{67}(b_u)$ 606.8
	$\nu_{16}(a_g)$ 406.3	$\nu_{42}(a_u)$ 1357.8	$\nu_{68}(b_u)$ 584.2
	$\nu_{17}(a_g)$ 395.3	$\nu_{43}(a_u)$ 1192.0	$\nu_{69}(b_u)$ 574.6
	$\nu_{18}(a_g)$ 320.7	$\nu_{44}(a_u)$ 1021.8	$\nu_{70}(b_u)$ 487.0
	$\nu_{19}(a_g)$ 311.6	$\nu_{45}(a_u)$ 911.9	$\nu_{71}(b_u)$ 473.6
	$\nu_{80}(a_g)$ 191.0	$\nu_{46}(a_u)$ 771.5	$\nu_{72}(b_u)$ 431.3
	$\nu_{21}(a_g)$ 82.5	$\nu_{47}(a_u)$ 762.5	$\nu_{73}(b_u)$ 418.3
	$\nu_{22}(b_g)$ 2160.9	$\nu_{48}(a_u)$ 664.0	$\nu_{74}(b_u)$ 398.8
	$\nu_{23}(b_g)$ 1813.0	$\nu_{49}(a_u)$ 584.2	$\nu_{75}(b_u)$ 241.2
	$\nu_{24}(b_g)$ 1351.3	$\nu_{50}(a_u)$ 544.3	$\nu_{76}(b_u)$ 153.9
	$\nu_{25}(b_g)$ 1247.6	$\nu_{51}(a_u)$ 477.2	$\nu_{77}(b_u)$ 114.0
	$\nu_{26}(b_g)$ 1009.4	$\nu_{52}(a_u)$ 455.4	$\nu_{78}(b_u)$ 75.0

Table 6S. Molecular Properties of structure E - $B_6H_6Li_2$ (D_{3d} , $^1A_{1g}$) (Fig.1) at the B3LYP/6-311++G** level of theory

Geometry:

Center Number	Atomic Simbol	Coordinates		
		X	Y	Z
1	Li	0.0000	0.0000	2.6311
2	B	0.0000	1.0040	0.6940
3	H	0.0000	1.9949	1.3790
4	B	0.8695	-0.5020	0.6940
5	H	1.7276	-0.9974	1.3790
6	B	-0.8695	-0.5020	0.6940
7	H	-1.7276	-0.9974	1.3790
8	Li	0.0000	0.0000	-2.6311
9	B	-0.8695	0.5020	-0.6940
10	H	-1.7276	0.9974	-1.3790
11	B	0.0000	-1.0040	-0.6940
12	H	0.0000	-1.9949	-1.3790
13	B	0.8695	0.5020	-0.6940
14	H	1.7276	0.9974	-1.3790

Other Properties:

	B3LYP/6-311++G**	
E _{total} , a.u.	-167.911433**	
NImag	0	
ZPE, kcal/mol	50.39599	
Frequencies	ν_1 (a _{1g}) 2524.3	ν_{15} (a _{1u}) 847.3
	ν_2 (a _{1g}) 1010.4	ν_{16} (a _{1u}) 453.3
	ν_3 (a _{1g}) 839.4	ν_{17} (a _{1u}) 105.2
	ν_4 (a _{1g}) 813.6	ν_{18} (a _{2u}) 2489.8
	ν_5 (a _{1g}) 646.4	ν_{19} (a _{2u}) 1027.4
	ν_6 (a _{1g}) 483.6	ν_{20} (a _{2u}) 682.6
	ν_7 (a _{1g}) 145.7	ν_{21} (a _{2u}) 523.4
	ν_8 (a _{1g}) 852.6	ν_{22} (a _{2u}) 133.1
	ν_9 (a _{1g}) 837.5	ν_{23} (e _u) 2488.2
	ν_{10} (a _{1g}) 118.5	ν_{24} (e _u) 1091.2
	ν_{11} (e _g) 2476.5	ν_{25} (e _u) 835.0
	ν_{12} (e _g) 871.0	ν_{26} (e _u) 722.0
	ν_{13} (e _g) 750.0	ν_{27} (e _u) 465.5
	ν_{14} (e _g) 859.0	

** - E_{total} (CCSD(T)/6-311++G**) = -167.280617