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Article

Arachno, Nido, and Closo Aromatic Isomers of the $Li_6B_6H_6$ Molecule

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We analyzed chemical bonding in low-lying isomers of the recently computationally predicted $B_6H_6Li_6$ molecule. According to our calculations the benzene-like $B_6H_6Li_6$ (D_{2h}, $^1A_{1g}$) arachno structure with the planar aromatic $B_6H_6^{6-}$ anion is the most stable one. A nido isomer with two aromatic $B_6H_6^{4-}$ (pentagonal pyramid) and Li_3^+ (triangular) moieties, which can be considered as derived from the global minimum structure through a two-electron intramolecular transfer from $B_6H_6^{6-}$ to three Li^+ cations, was found to be 10.7 kcal/mol higher in energy. A closo isomer with three aromatic moieties (octahedral $B_6H_6^{2-}$ and two Li_3^+) was found to be 31.3 kcal/mol higher in energy than the global minimum. Another isomer with three aromatic moieties (two $B_3H_3^{2-}$ and Li_3^+) was found to be substantially higher in energy (74.4 kcal/mol). Thus, the intramolecular electron transfers from the highly charged $B_6H_6^{6-}$ anion to cations are not favorable for the $B_6H_6Li_6$ molecule, even when a formation of three-dimensional aromatic $B_6H_6^{2-}$ anion and two σ-aromatic Li_3^+ cations occurs in the closo isomer.

1. Introduction

In our recent work[1] we computationally predicted a new class of aromatic all-boron compounds such as $B_6H_6Li_6$ (D_{2h}, $^1A_{1g}$), $B_5H_5Li_6$ (C_s, $^1A'$), $B_7H_7Li_6$ (C_1, ^1A), and $B_{10}H_8Li_{10}$ (D_{2h}, ^1A_g) which are isoelectronic to their classical aromatic carbon analogues C_6H_6, $C_5H_5^-$, $C_7H_7^+$, and $C_{10}H_8$, respectively. Independently Fehlner and coauthors prepared sandwich complexes of rhenium with planar chlorinated boranes containing 5 and 6 boron atoms.[2,3] These new species can be considered as derived from deltahedral boranes[4−14] through many-electron reductions. Inorganic salts $M_2B_nH_n$ (M = alkali metal atoms) containing *closo*-boranes, $B_nH_n^{2-}$, are highly stable compounds and their stability was attributed to their three-dimensional aromaticity.[9−16] In spite of that, we predicted that the four-electron reduction of $B_6H_6^{2-}$ to $B_6H_6^{6-}$ in the gas-phase reaction between $B_6H_6Li_2$ and Li_4 is highly exothermic ($\Delta E = -53$ kcal/mol at the CCSD(T)/6-311++G** level of theory). Formation of the six classical two-center two-electron B−B σ-bonds, together with the three π-bonds and their resonance, provides the extra stability for the planar aromatic $B_6H_6^{6-}$ structure inside of the $B_6H_6Li_6$ molecule. In our work[1] we also computationally found many low-lying isomers, which are very interesting species from a chemical bonding point of view, and they are at the center of this Article.

In this work we consider low-lying isomers only for the $B_6H_6Li_6$ molecule, while similar analysis can be made for other all-boron aromatic $B_5H_5Li_6$ (C_s, $^1A'$), $B_7H_7Li_6$ (C_1, ^1A) and $B_{10}H_8Li_{10}$ (D_{2h}, ^1A_g) molecules.

The low-lying isomers found for $B_6H_6Li_6$ are presented in Figure 1 (other alternative structure of $B_6H_6Li_6$ studied in this work are summarized in the Supporting Information). Their geometries, harmonic frequencies and relative energies

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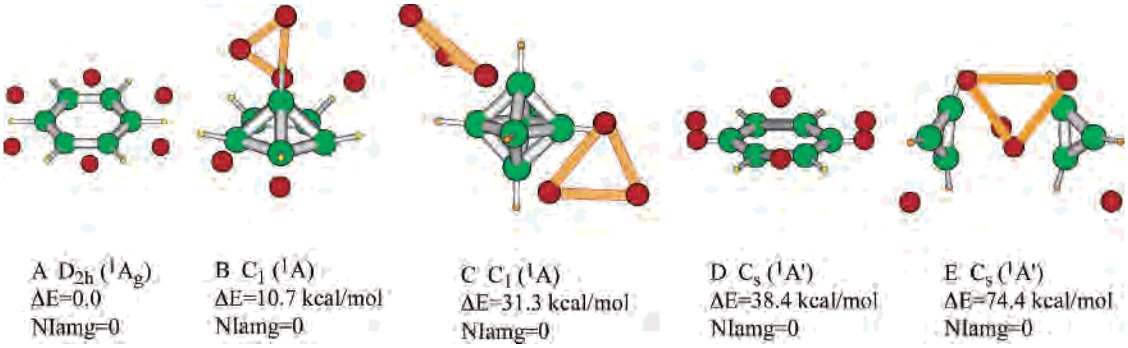
A D_{2h} (^1A_g)
ΔE=0.0
NImg=0

B C_1 (^1A)
ΔE=10.7 kcal/mol
NImg=0

C C_1 (^1A)
ΔE=31.3 kcal/mol
NImg=0

D C_s ($^1A'$)
ΔE=38.4 kcal/mol
NImg=0

E C_s ($^1A'$)
ΔE=74.4 kcal/mol
NImg=0

Figure 1. Low-lying isomers of $B_6H_6Li_6$ (B3LYP/6-311+G* level of theory).

Table 1. Molecular Properties of the Global Minimum Structure A of $B_6H_6Li_6$ (D_{2h}, ^1A_g) (Figure 1)

	B3LYP/6-311++G**		CASSCF(8,8)/6-311++G**		MP2/6-311++G**
E_{total}, a.u.	−198.077083[a]		−196.4171543		−196.3185709
ZPE, kcal/mol	55.73372		58.00506		*b*
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	*b*
	ν_2 (a_g) 1834.6	ν_{26} (a_u) 374.1	ν_2 (a_g) 1836.9	ν_{26} (a_u) 357.0	*b*
	ν_3 (a_g) 1234.1	ν_{27} (a_u) 53.9	ν_3 (a_g) 1331.7	ν_{27} (a_u) 69.9	*b*
	ν_4 (a_g) 1080.1	ν_{28} (b_{1u}) 706.9	ν_4 (a_g) 1152.2	ν_{28} (b_{1u}) 777.7	*b*
	ν_5 (a_g) 732.1	ν_{29} (b_{1u}) 554.9	ν_5 (a_g) 747.8	ν_{29} (b_{1u}) 596.4	*b*
	ν_6 (a_g) 518.2	ν_{30} (b_{1u}) 432.4	ν_6 (a_g) 532.4	ν_{30} (b_{1u}) 423.8	*b*
	ν_7 (a_g) 463.3	ν_{31} (b_{1u}) 343.3	ν_7 (a_g) 470.4	ν_{31} (b_{1u}) 370.3	*b*
	ν_8 (a_g) 413.2	ν_{32} (b_{1u}) 61.1	ν_8 (a_g) 411.9	ν_{32} (b_{1u}) 65.1	*b*
	ν_9 (a_g) 342.4	ν_{33} (b_{2u}) 2173.7	ν_9 (a_g) 356.6	ν_{33} (b_{2u}) 2197.4	*b*
	ν_{10} (b_{1g}) 2149.5	ν_{34} (b_{2u}) 1394.5	ν_{10} (b_{1g}) 2171.0	ν_{34} (b_{2u}) 1470.0	*b*
	ν_{11} (b_{1g}) 1378.2	ν_{35} (b_{2u}) 1199.1	ν_{11} (b_{1g}) 14.52.0	ν_{35} (b_{2u}) 1265.5	*b*
	ν_{12} (b_{1g}) 1251.8	ν_{36} (b_{2u}) 999.9	ν_{12} (b_{1g}) 1343.2	ν_{36} (b_{2u}) 1029.1	*b*
	ν_{13} (b_{1g}) 991.1	ν_{37} (b_{2u}) 902.3	ν_{13} (b_{1g}) 1023.4	ν_{37} (b_{2u}) 914.5	*b*
	ν_{14} (b_{1g}) 646.7	ν_{38} (b_{2u}) 521.4	ν_{14} (b_{1g}) 656.8	ν_{38} (b_{2u}) 564.5	*b*
	ν_{15} (b_{1g}) 510.1	ν_{39} (b_{2u}) 416.0	ν_{15} (b_{1g}) 528.3	ν_{39} (b_{2u}) 517.4	*b*
	ν_{16} (b_{1g}) 384.9	ν_{40} (b_{2u}) 316.7	ν_{16} (b_{1g}) 404.1	ν_{40} (b_{2u}) 328.8	*b*
	ν_{17} (b_{2g}) 748.2	ν_{41} (b_{3u}) 2158.6	ν_{17} (b_{2g}) 820.2	ν_{41} (b_{3u}) 2180.5	*b*
	ν_{18} (b_{2g}) 620.3	ν_{42} (b_{3u}) 1825.3	ν_{18} (b_{2g}) 678.7	ν_{42} (b_{3u}) 1831.3	*b*
	ν_{19} (b_{2g}) 517.0	ν_{43} (b_{3u}) 1267.6	ν_{19} (b_{2g}) 547.5	ν_{43} (b_{3u}) 1359.3	*b*
	ν_{20} (b_{2g}) 428.5	ν_{44} (b_{3u}) 825.1	ν_{20} (b_{2g}) 433.2	ν_{44} (b_{3u}) 846.8	*b*
	ν_{21} (b_{2g}) 62.8	ν_{45} (b_{3u}) 722.7	ν_{21} (b_{2g}) 79.9	ν_{45} (b_{3u}) 760.5	*b*
	ν_{22} (b_{3g}) 612.0	ν_{46} (b_{3u}) 609.1	ν_{22} (b_{3g}) 666.5	ν_{46} (b_{3u}) 607.2	*b*
	ν_{23} (b_{3g}) 435.3	ν_{47} (b_{3u}) 395.5	ν_{23} (b_{3g}) 433.6	ν_{47} (b_{3u}) 407.6	*b*
	ν_{24} (b_{3g}) 82.3	ν_{48} (b_{3u}) 348.0	ν_{24} (b_{3g}) 85.9	ν_{48} (b_{3u}) 399.3	*b*

[a] E_{total} (CCSD(T)/6-311++G**) = −197.1957259. [b] Frequencies were not calculated at this level of theory.

have been determined at the hybrid B3LYP[17] level of theory using the polarized split-valence (6-311++G**)[18] basis sets. Molecular properties of the global minimum isomer also have been obtained at the CASSCF(8,8)[19] and at the MP2[20] levels of theory. Calculated molecular properties of isomers A, B, and C are presented in Tables 1 and 2 (properties of higher-energy isomers are given in the Supporting Information). Natural population analysis (NPA)[21] was performed for all discussed structures. All calculations were performed using the Gaussian 03 program[22] on 63-node Birch−Retford Beowulf cluster computer built at USU by K. A. Birch and B. P. Retford. Molecular orbitals' pictures were made using the MOLDEN3.4 program.[23]

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Table 2. Molecular Properties of Low-Lying Isomers of $B_6H_6Li_6$ (Figure 1) at the B3LYP/6-311++G** Level of Theory

	isomer B, C_1 ($^1A_1$)			isomer C, C_1 ($^1A_1$)		
E_{total}, a.u.	−198.0600761			−198.027177		
ZPE, kcal/mol	55.91281			54.948		
			Frequencies			
	ν_1 2346.8	ν_1 883.7	ν_3 475.0	ν_1(a′) 2568.3	ν_{17} (a′) 842.9	ν_{33} (a″) 333.8
	ν_2 2318.8	ν_{18} 867.6	ν_{34} 431.9	ν_2 (a′) 2547.2	ν_{18} (a′) 836.1	ν_{34} (a″) 329.7
	ν_3 2289.1	ν_{19} 837.4	ν_{35} 423.9	ν_3 (a′) 2541.7	ν_{19} (a′) 808.3	ν_{35} (a″) 309.5
	ν_4 2281.3	ν_{80} 826.0	ν_{36} 383.9	ν_4 (a′) 2538.6	ν_{80} (a′) 799.2	ν_{36} (a″) 303.0
	ν_5 2260.5	ν_{21} 812.3	ν_{37} 374.7	ν_5 (a′) 2525.5	ν_{21} (a′) 775.0	ν_{37} (a″) 242.7
	ν_6 2228.6	ν_{22} 759.1	ν_{38} 351.6	ν_6 (a′) 2518.2	ν_{22} (a′) 759.5	ν_{38} (a″) 220.2
	ν_7 1180.6	ν_{23} 713.5	ν_{39} 339.2	ν_7 (a′) 1110.7	ν_{23} (a′) 736.6	ν_{39} (a″) 185.3
	ν_8 1110.7	ν_{24} 674.8	ν_{40} 283.4	ν_8 (a′) 1085.0	ν_{24} (a′) 727.1	ν_{40} (a″) 179.7
	ν_9 1099.2	ν_{25} 645.5	ν_{41} 273.2	ν_9 (a′) 1056.6	ν_{25} (a′) 709.0	ν_{41} (a″) 177.1
	ν_{10} 1030.5	ν_{26} 641.8	ν_{42} 228.3	ν_{10} (a′) 999.7	ν_{26} (a′) 701.8	ν_{42} (a″) 169.1
	ν_{11} 1021.0	ν_{27} 616.8	ν_{43} 201.4	ν_{11} (a′) 947.4	ν_{27} (a′) 690.5	ν_{43} (a″) 132.1
	ν_{12} 996.5	ν_{28} 600.9	ν_{44} 163.7	ν_{12} (a′) 946.7	ν_{28} (a″) 495.9	ν_{44} (a″) 112.5
	ν_{13} 934.2	ν_{29} 546.8	ν_{45} 136.1	ν_{13} (a′) 907.6	ν_{29} (a″) 469.8	ν_{45} (a″) 89.3
	ν_{14} 915.0	ν_{30} 541.5	ν_{46} 116.4	ν_{14} (a′) 884.8	ν_{30} (a″) 455.5	ν_{46} (a″) 67.9
	ν_{15} 907.9	ν_{31} 519.4	ν_{47} 73.9	ν_{15} (a′) 864.7	ν_{31} (a″) 417.9	ν_{47} (a″) 27.3
	ν_{16} 889.0	ν_{32} 507.0	ν_{48} 51.8	ν_{16} (a′) 854.9	ν_{32} (a″) 390.9	ν_{48} (a″) 12.6

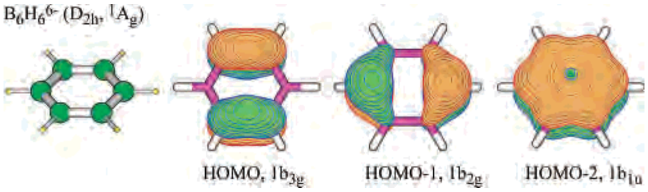

Figure 2. π-Molecular orbitals of $B_6H_6^{6-}$ fragment of $B_6H_6Li_6$ isomer A.

2. Chemical Bonding in the $B_6H_6Li_6$ (D_{2h}, $^1A_{1g}$) Arachno Global Minimum Isomer A

The (D_{2h}, $^1A_{1g}$) global minimum isomer of $B_6H_6Li_6$ was found to have the $1a_g^2 1b_{3u}^2 1b_{2u}^2 2a_g^2 1b_{1g}^2 2b_{3u}^2 3a_g^2 3b_{3u}^2 2b_{2u}^2 3b_{2u}^2 1b_{1u}^2 2b_{1g}^2 4a_g^2 1b_{2g}^2 1b_{3g}^2$ electronic configuration. It contains a highly charged $B_6H_6^{6-}$ core, which is surrounded and stabilized by 6 Li^+ cations. In the $B_6H_6^{6-}$ anion, six classical two-center two-electron B−B σ-bonds and the resonance of the three two-center two-electron π-bonds are responsible for chemical bonding. Apparently, the formation of the six B−B σ-bonds, which are rather strong (D_e(B−B) = 101 kcal/mol from the dissociation of B_2H_4 into two BH_2 fragments), together with formation of the three π-bonds and their resonance, provides the extra stability for the aromatic $B_6H_6^{6-}$ structure in spite its highly negative charge. The three π-molecular orbitals containing 6 electrons, which are shown in Figure 2, make this system aromatic and similar to benzene. Completely bonding HOMO-2 and the partially bonding HOMO and HOMO-1 of $B_6H_6Li_6$ have exactly the same form as the π-molecular orbitals of benzene. Li^+ countercations stabilize the −6 charge on the borane. A substantial charge transfer from the Li atoms (Q(Li) = +0.92 − +0.97 e, calculated using the natural population analysis) provides the required number of electrons on the B_6H_6 part and populates the depicted molecular orbitals making the system π-aromatic. The isomer D has the same $B_6H_6^{6-}$ core as the global minimum and differs by a different location of Li^+ countercations (one above the $B_6H_6^{6-}$ plane and five others in this plane). Apparently the location of the six Li^+ cations in the global minimum structure A is more favorable. Both isomers A and D can be classified as *arachno*-boranes,[4,10−13] because they can be formally assigned to the B_nH_{n+6} class with $n = 6$ and six H^+ being removed. The framework electron count satisfies the $(2n + 6)$ rule.[10,11,24]

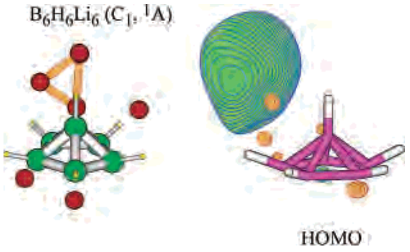

Figure 3. The HOMO (completely bonding σ-molecular orbital of Li_3^+) of the $B_6H_6Li_6$ isomer B.

3. Chemical Bonding in the $B_6H_6Li_6$ (C_1, ^1A) Nido Isomer B

The second isomer B (Figure 1) was found to be 10.7 kcal/mol higher than the global minimum at the B3LYP/6-311++G** level of theory. Careful examination of the isomer B of $B_6H_6Li_6$ reveals the presence of a triangular moiety Li_3^+ coordinated to the $B_6H_6^{4-}$ tetraanion with the three other Li^+ cations coordinated to the tetraanion (Figure 3).

Thus, in this isomer a two-electron transfer occurs from the $B_6H_6^{6-}$ hexaanion to three Li^+ cations followed by the formation of a new Li_3^+ moiety, which makes this structure differ from the global minimum. The Li_3^+ unit was shown to be a σ-aromatic system.[25] The HOMO in the isomer B (Figure 3) is a completely bonding σ-aromatic molecular orbital of Li_3^+ fragment. The reduction of $B_6H_6^{6-}$ into $B_6H_6^{4-}$ leads to a structural rearrangement of the planar hexagon $B_6H_6^{6-}$ into the aromatic pentagonal pyramid $B_6H_6^{4-}$. The aromaticity of the $B_6H_6^{4-}$ can be clearly seen from molecular orbitals shown in Figure 4.

The central B atom of the pyramid donates electrons to the π-system of the base, thus providing the required number of electrons for populating these three peculiar π-molecular orbitals and making the system π-aromatic. The $B_6H_6^{4-}$ core

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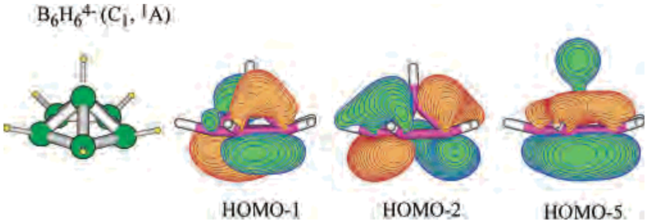

Figure 4. Aromatic molecular orbitals of $B_6H_6^{4-}$ fragment in the $B_6H_6Li_6$ isomer B.

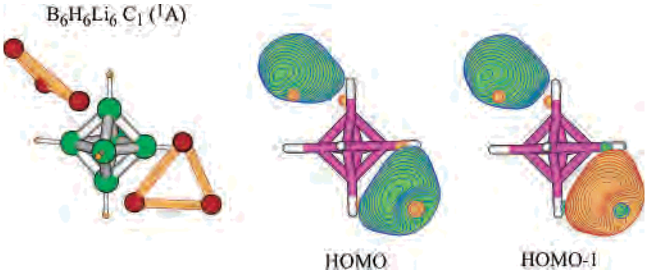

Figure 5. HOMO and HOMO-1 of the isomer C of $B_6H_6Li_6$: linear combinations of the completely bonding σ-molecular orbitals of the Li_3^+ fragments.

of the cluster is a *nido*-borane according to the B_nH_{n+4} classification for the nido compounds[4,10-13] (for $n = 6$ and four protons being removed). The departure of two electrons from the benzene-like $B_6H_6^{6-}$ moiety and the formation of the σ-aromatic Li_3^+ cation and aromatic *nido*-$B_6H_6^{4-}$ moiety in the $B_6H_6Li_6$ molecule do not compensate the loss of the stability, because the nido isomer B is less stable than the arachno isomer A by 10.7 kcal/mol.

4. Chemical Bonding in the $B_6H_6Li_6$ (C_1, ^1A) Closo Isomer C

Four-electron oxidation of the $B_6H_6^{6-}$ unit with the simultaneous formation of the $B_6H_6^{2-}$ octahedral unit and the formation of two σ-aromatic Li_3^+ triangular units yields the isomer C (Figure 5). The isomer C was found to be 31.3 kcal/mol above the global minimum. The natural population analysis supports the presence of two distinct aromatic Li_3^+ units coordinated to the opposing sides of the $B_6H_6^{2-}$ octahedral cluster. As one can see, HOMO and HOMO-1 in the isomer C are simply linear combinations of the σ-bonding aromatic molecular orbitals in the Li_3^+ fragments. The $B_6H_6^{2-}$ dianion is the *closo*-borane.[4,10-13]

The stability of the $B_6H_6^{2-}$ octahedron comes from two types of bonding: peripheral, constructed by the overlap of the 6 pairs of the p_x,p_y-tangential B orbitals over the two-dimensional faces of the quasi-octahedron, and global, formed by the global mutual overlap of the 6 sp_z-hybrid B orbitals.[10,13] The latter type of bonding is responsible for the symmetry, special stability, and three-dimensional aromaticity of the species. Figure 6 demonstrates the set of molecular orbitals responsible for the bonding within the quasi-octahedral $B_6H_6^{2-}$ unit. The global bonding and three-dimensional aromaticity of the species are performed by HOMO-5, HOMO-6, HOMO-7, and HOMO-10. HOMO-10 is a completely bonding molecular orbital formed by the globally overlapping sp_z-hybridized atomic orbitals of all 6 boron atoms. Partially bonding HOMO-5, HOMO-6, and

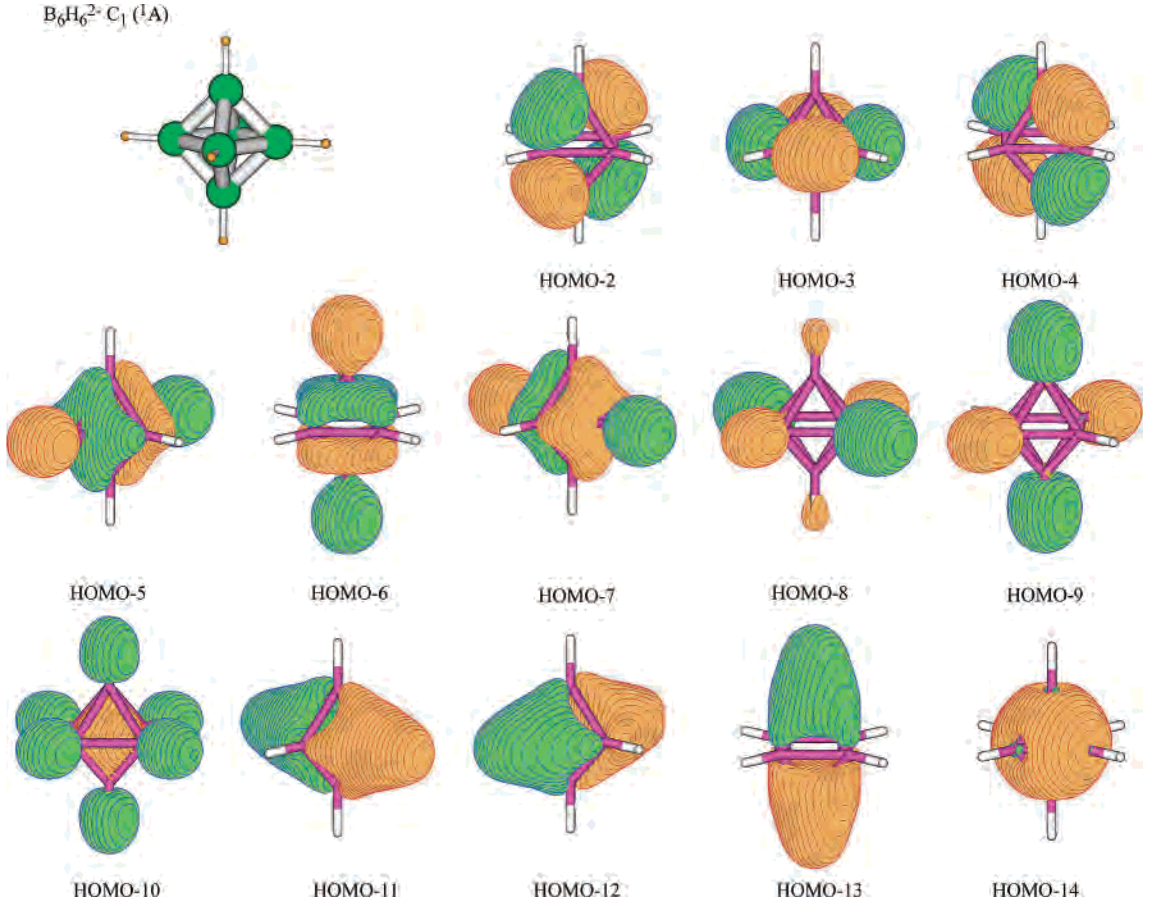

Figure 6. Global overlap molecular orbitals in the $B_6H_6Li_6$ isomer C.

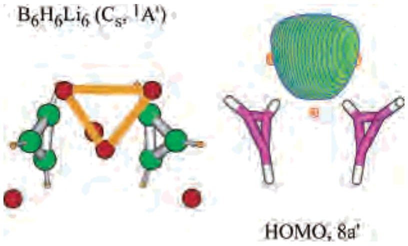

Figure 7. Molecular orbital of the Li_3^+ fragment in the $B_6H_6Li_6$ isomer E: HOMO.

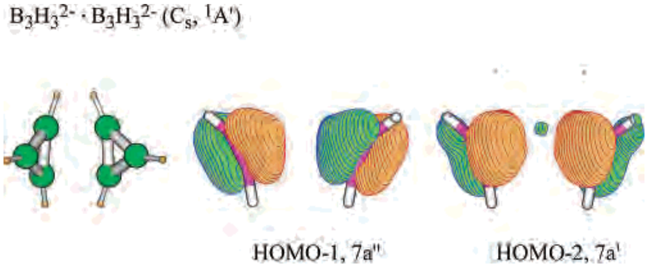

Figure 8. HOMO-1 and HOMO-2 in the isomer E of $B_6H_6Li_6$.

HOMO-7, which would belong to the triply degenerate set in the perfect octahedral species, are formed by sp_z-hybridized atomic orbitals of 2 boron atoms opposing each other, and 4 tangential p-atomic orbitals of the remaining 4 boron atoms of the system.

Complete occupations of the nondegenerate bonding HOMO-10 and quasi-degenerate partially bonding HOMO-5, HOMO-6, and HOMO-7 lead to the octahedral structure of the borane core having equalized bond lengths. Eight electrons thus available for the global type of chemical bonding cannot be localized as classical 2c−2e bonds. Consequently, the global bonding within the system has a distinct delocalized character, and the borane is three-dimensionally aromatic.

5. Chemical Bonding in the $B_6H_6Li_6$ (C_s, $^1A'$) Isomer E

The isomer E, which consists of two separate $B_3H_3^{2-}$ fragments surrounded by the Li_3^+ cluster and three Li^+ cations, was found to be 74.4 kcal/mol less stable than the global minimum. HOMO in the isomer E is the aromatic σ-bonding molecular orbital of the Li_3^+ species (Figure 7).

Two $B_3H_3^{2-}$ units have molecular orbitals similar to those in $C_3H_3^+$, which is a π-aromatic organic molecule. Thus, $B_3H_3^{2-}$ has 2 π-electrons and obeys the $(4n + 2)$ Huckel rule for π-aromatic systems. HOMO-1 and HOMO-2 in the isomer are linear combinations of completely bonding π-molecular orbitals of the individual $B_3H_3^{2-}$ fragments (Figure 8).

Therefore, the isomer E consists of three aromatic fragments: two $B_3H_3^{2-}$ and one Li_3^+. However, because it is substantially higher in energy than the closo, nido, or arachno isomers, it shows that the larger electron delocalization in isomers A, B, and C makes the latter isomers more stable.

6. Conclusions

One may think that, in the $B_6H_6Li_6$ molecule, the closo structure C with the highly stable spherically aromatic dianion $B_6H_6^{2-}$ should be substantially more stable than the arachno structure A with the benzene-like $B_6H_6^{6-}$ anion. First, the $B_6H_6^{2-}$ dianion carries fewer extra charges than the $B_6H_6^{6-}$ hexaanion, thus reducing enormous Coulomb repulsion in the boron core. Second, the spherical aromaticity of $B_6H_6^{2-}$ is known to make very stable $M_2B_6H_6$ (M = alkali metal) salts. Third, four electrons removed from the boron core go to form two σ-aromatic Li_3^+ moieties, thus providing additional stability for the closo isomer C. Yet, according to our calculations the benzene-like $B_6H_6Li_6$ (D_{2h}, $^1A_{1g}$) arachno structure with the aromatic planar $B_6H_6^{6-}$ anion is the most stable. The closo isomer with three aromatic moieties ($B_6H_6^{2-}$ and two Li_3^+) was found to be 31.3 kcal/mol higher in energy than the global minimum. Moreover, the nido isomer B with two aromatic $B_6H_6^{4-}$ and Li_3^+ moieties, which can be considered as derived from the global minimum through two-electron intramolecular transfer from $B_6H_6^{6-}$ to three Li^+ cations, was found to be second in stability, being 10.7 kcal/mol higher in energy than the global minimum.

When the B_6H_6 borane core is split into two aromatic $B_3H_3^{2-}$ moieties, the resulting structure E was found being substantially higher in energy (74.4 kcal/mol).

It is hard for theoreticians to speculate about the way to synthesize described compounds, but we would suggest two possible approaches to the synthetic problem. The first one is to lithiate $B_6H_6Li_2$ salt under appropriate conditions. The second one is to perform an electrochemical reduction of this salt. An alternative approach has been already used by Fehlner and co-workers,[2,3] in which instead of complete charge transfer from cations to anions they incorporated a B_6H_6 structural unit into a sandwich structure between two rhenium atoms. The success of Fehlner and co-workers in making planar B_6H_6 compounds gives us hope that our $B_6H_6Li_6$ isomers also can be synthesized.

To summarize, we would like to stress that, according to our calculations of the $B_6H_6Li_6$ isomers, the two-dimensional aromaticity wins the competition with three-dimensional aromaticity in this particular compound. We hope that our analysis of chemical bonding in the $B_6H_6Li_6$ isomers will help to understand better the competition between two- and three-dimensional aromaticities in inorganic chemistry.

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Supporting Information Available: A picture of all found low-lying isomers of $B_6H_6Li_6$, calculated molecular properties of all low-lying $B_6H_6Li_6$ isomers discussed in the paper (geometries, vibrational frequencies, and natural atomic charges), and pictures of complete sets of molecular orbitals of all isomers. This material is available free of charge via the Internet at http://pubs.acs.org.

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