Molecular Wheel B_8^{2-} as a New Inorganic Ligand. Photoelectron Spectroscopy and Ab Initio Characterization of LiB_8^-

Anastassia N. Alexandrova*, Hua-Jin Zhai**, Lai-Sheng Wang**, and Alexander I. Boldyrev*

*Department of Chemistry and Biochemistry, Utah State University, Logan, Utah 84322-0300 (USA). E-mail: bodyrev@cc.usu.edu

**Department of Physics, Washington State University, 2710 University Drive, Richland, WA 99352 (USA) and W. R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, MS K8-88, P. O. Box 999, Richland, WA 99352 (USA). E-mail: ls.wang@pnl.gov

Supporting Information

Figure S1. Alternative structures of LiB_8^- at the B3LYP/6-311+G* level of theory.

Figure S2. Molecular orbitals of the LiB_8^- (C_{7v} , 1A_1) global minimum isomer.

Table S1. Calculated properties of the LiB_8^- (C_{7v} , 1A_1) global minimum structure at the B3LYP/6-311+G* level of theory.

I, C_{7v} (1A_1)
 $\Delta E=0.0$
 NImag=0

II, C_{2v} (1A_1)
 $\Delta E=32.3$ kcal/mol
 NImag=1

III, C_{2v} (1A_1)
 $\Delta E=38.7$ kcal/mol
 NImag=2

IV, C_1 (1A)
 $\Delta E=45.4$ kcal/mol
 NImag=0

V, C_s ($^1A'$)
 $\Delta E=46.6$ kcal/mol
 NImag=1

VI, C_{6v} ($^1A_{1g}$)
 $\Delta E=54.7$ kcal/mol
 NImag=2

VII, C_s ($^1A'$)
 $\Delta E=$ kcal/mol
 NImag=

VIII, C_s ($^1A'$)
 $\Delta E=63.1$ kcal/mol
 NImag=0

IX, C_2 (1A)
 $\Delta E=63.7$ kcal/mol
 NImag=0

X, C_2 (1A)
 $\Delta E=66.2$ kcal/mol
 NImag=0

XI, C_{2v} (1A_1)
 $\Delta E=68.7$ kcal/mol
 NImag=1

XII, C_{2v} (1A_1)
 $\Delta E=77.0$ kcal/mol
 NImag=1

Figure S1.

Figure S2.

Table S1.

E_{total} , a.u.	-206.296837
$R(\text{Li-B}_2)$	2.040 Å
$R(\text{Li-B}_{3,4,5,6,7})$	2.494 Å
$\angle(\text{Li-B}_2\text{-B}_{3,4,5,6,7})$	80.78°
NImag	0
ZPE, kcal/mol	20.633
$\omega_1(a_1)$, cm^{-1}	819.0 (0.2)
$\omega_2(a_1)$, cm^{-1}	669.7 (71.3)
$\omega_3(a_1)$, cm^{-1}	381.8 (20.9)
$\omega_4(a_1)$, cm^{-1}	208.6 (3.4)
$\omega_5(a_1)$, cm^{-1}	204.8 (3.4)
$\omega_6(a_2)$, cm^{-1}	343.7 (0.0)
$\omega_7(e_1)$, cm^{-1}	971.2 (10.8)
$\omega_8(e_1)$, cm^{-1}	602.1 (8.9)
$\omega_9(e_3)$, cm^{-1}	1375.0 (0.0)
$\omega_{10}(e_3)$, cm^{-1}	1253.3 (0.0)
$\omega_{11}(e_3)$, cm^{-1}	491.7 (0.0)
$\omega_{12}(e_3)$, cm^{-1}	343.7 (0.0)
$\omega_{13}(e_3)$, cm^{-1}	428.2 (0.0)
$\omega_{14}(e_3)$, cm^{-1}	609.2 (0.0)

* Infrared intensities are shown in parentheses.