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Electronic Supplementary Information

Singlet and triplet states of the sandwich-type Be_2B_6 and $Be_2B_7^+$ clusters. A test for electron counting rules of aromaticity

Slađana Đorđević, Slavko Radenković*

University of Kragujevac, Faculty of Science, P. O. Box 60, 34000 Kragujevac, Serbia

*Corresponding author: slavkoradenkovic@kg.ac.rs

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a)   σ   π

SOMO ($2e_1'$)   SOMO' ($2e_1'$)   HOMO-1 ($1e_1''$)   HOMO-1 ($1e_1''$)

HOMO-2 ($1a_1'$)   HOMO-4 ($1a_2''$)

b)   σ   π

HOMO ($8a_1$)   HOMO-1 ($3b_1$)   HOMO-1' ($1a_2$)

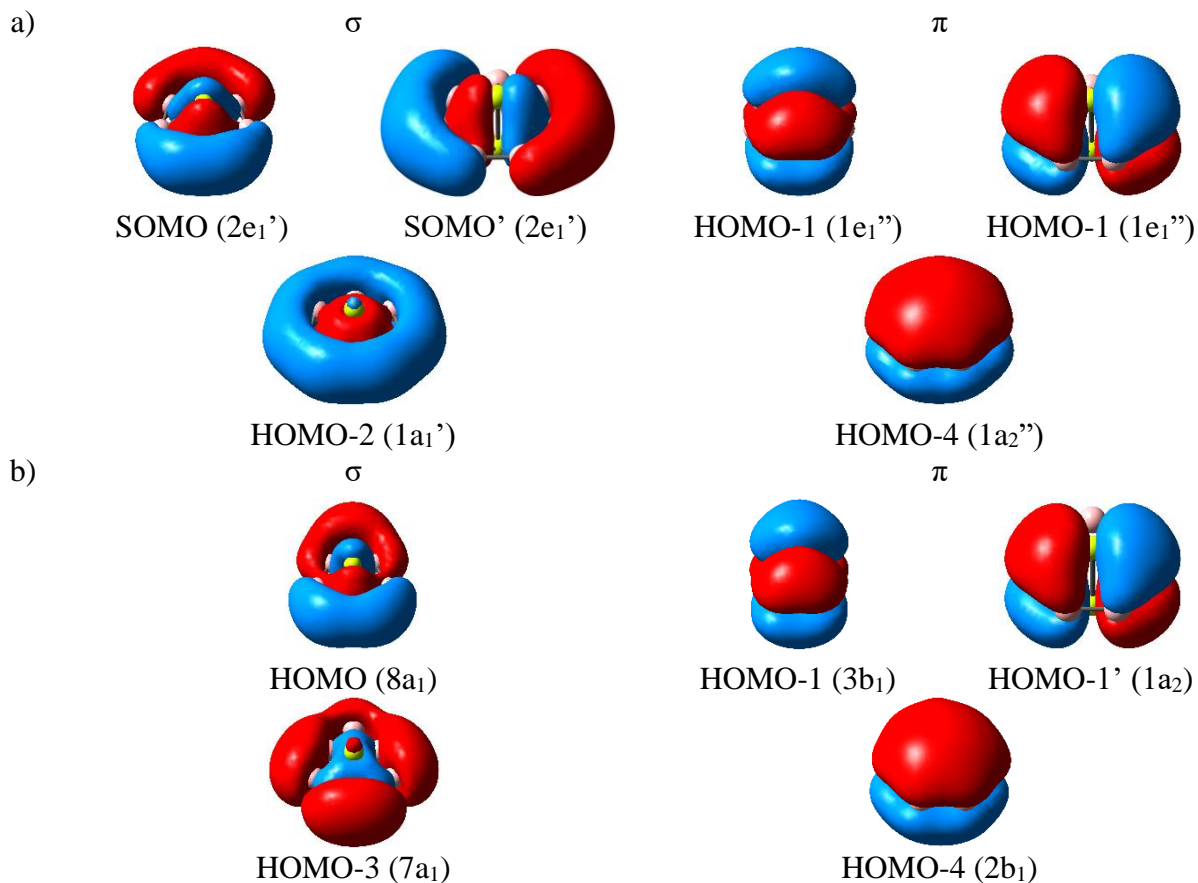HOMO-3 ($7a_1$)   HOMO-4 ($2b_1$)

Figure S1. a) σ and π occupied canonical molecular spin orbitals for **2T** obtained at the UB3LYP/def2-TZVP level; b) σ and π occupied canonical molecular orbitals for **2S** obtained at the RB3LYP/def2-TZVP level of theory.

1T **1S** **2T** **2S**
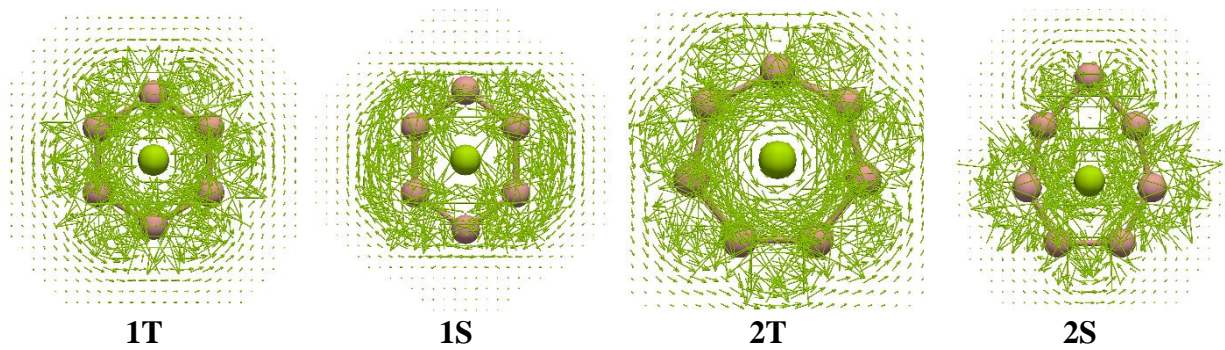
Figure S2. Total current density maps calculated 1 bohr above boron planes. Other details same as in Figure 3.
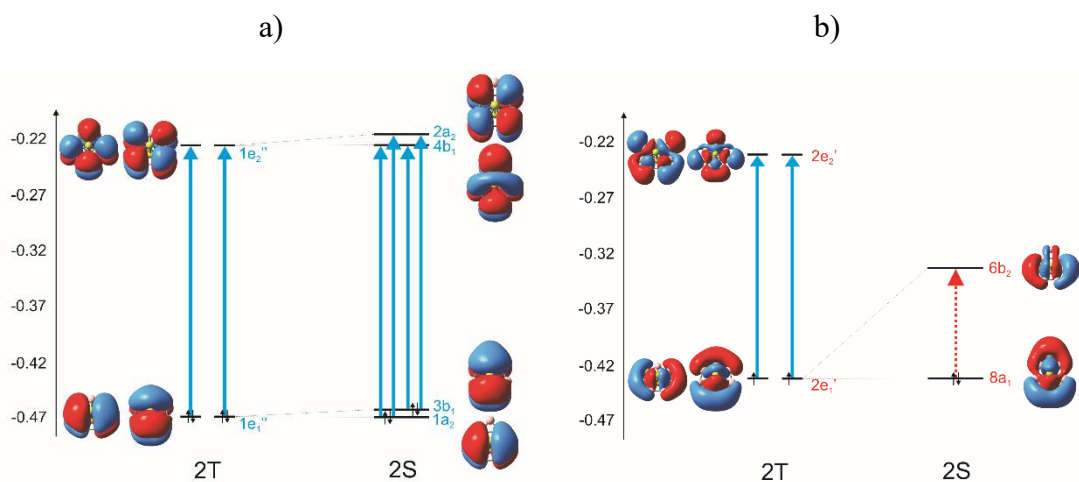
Figure S3. π (a) and σ (b) frontier orbital energy levels (in au) of **2T** and **2S** obtained at the B3LYP/def2-TZVP level of theory. Full (blue) arrows represent the main translational transitions and dashed (red) arrows represent the main rotational transitions.
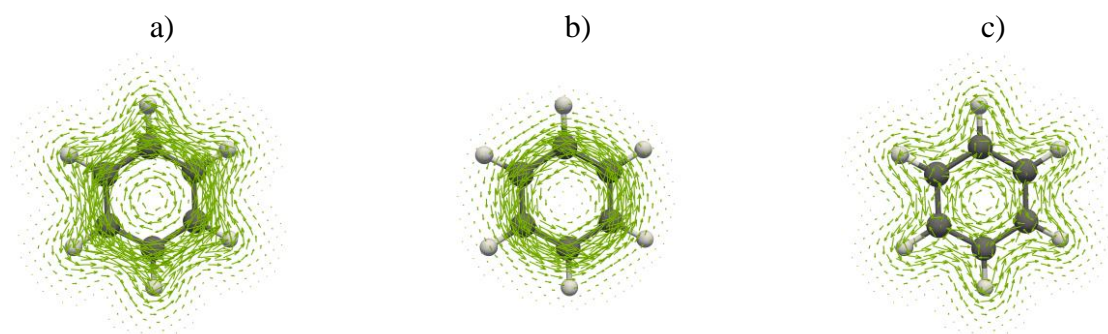
Figure S4. Maps of total current densities (a), π electron current densities (b) and σ electron current densities (c) of benzene calculated 1 bohr above the molecular plane. Other details same as in Figure 3.

Table S1. Bond current strengths (in nA T^{-1}) for the symmetry-unique bonds in **3T**, **3S** and benzene.

	3T				**3S**				benzene		
bond	total	σ	π	bond	total	σ	π	bond	total	σ	π
B1-B2	8.2	3.2	4.5	B1-B2	5.5	1.5	3.1	C1-C2	4.47	4.52	-0,05
				B2-B3	2.6	-2.9	4.4				
				B3-B4	3.3	-2.2	4.4				
				B4-B5	3.9	-0.9	4.1				

Table S2. Cartesian coordinates and energy (in au) for **1T**, **1S**, **2T**, **2S**, **3T** and **3S** at the B3LYP/def2-TZVP level of theory

1T		-178.44668804		**1S**		-178.43340350
0 3				0 1		
5	0.00000000	1.56850000	0.00000000	5	-0.82094500	1.24402500	-0.00003700
5	-1.35836100	0.78425000	0.00000000	5	-1.71448701	0.00010600	-0.00001200
5	-1.35836100	-0.78425000	0.00000000	5	-0.82114100	-1.24395400	-0.00003400
5	0.00000000	-1.56850000	0.00000000	5	0.82097100	-1.24410700	0.00003300
5	1.35836100	-0.78425000	0.00000000	5	1.71440000	-0.00010700	0.00002900
5	1.35836100	0.78425000	0.00000000	5	0.82116600	1.24402900	0.00003500
4	0.00000000	0.00000000	1.10153701	4	-0.00008000	0.00000600	1.13793200
4	0.00000000	0.00000000	-1.10153701	4	0.00012400	0.00000500	-1.13795000

2T		-203.04051911		**2S**		-203.02299698
1 3				1 1		
5	0.00000000	1.77342901	0.00000000	5	2.30472300	-0.00020300	-0.00004600
5	-0.76946200	-1.59780400	0.00000000	5	-1.72151001	0.76275400	-0.00003200
5	-1.72896500	-0.39462500	0.00000000	5	-0.37968400	1.51962800	-0.00006200
5	1.72896500	-0.39462500	0.00000000	5	-0.38000400	-1.51952800	0.00004200
5	1.38652301	1.10571500	0.00000000	5	1.12231201	-0.97529300	0.00000500
5	-1.38652301	1.10571500	0.00000000	5	1.12254100	0.97518300	0.00004200
5	0.76946200	-1.59780400	0.00000000	5	-1.72178300	-0.76259300	0.00004300
4	0.00000000	0.00000000	1.07698300	4	-0.21658600	0.00012900	1.15991600
4	0.00000000	0.00000000	-1.07698300	4	-0.21665600	-0.00006400	-1.15990800

3T		-227.39350083		**3S**		-227.38824824
2 3				2 1		
5	-1.85434700	0.76729700	0.00000000	5	-0.41931300	-1.98350500	0.00000000
5	-1.85434700	-0.76729700	0.00000000	5	1.10769500	-1.85972800	0.00000000
5	-0.76719900	-1.85038100	0.00000000	5	1.94310400	-0.57555500	0.00000000
5	0.76719900	-1.85038100	0.00000000	5	1.45642500	0.88745500	0.00000000
5	1.85434700	-0.76729700	0.00000000	5	0.08312000	1.65008500	0.00000000
5	1.85434700	0.76729700	0.00000000	5	-1.34027100	2.24947900	0.00000000
5	0.76719900	1.85038100	0.00000000	5	-1.49019100	0.71236600	0.00000000
5	-0.76719900	1.85038100	0.00000000	5	-1.47356000	-0.85844100	0.00000000
4	0.00000000	0.00000000	1.09706600	4	0.08312000	-0.13884700	1.13869200
4	0.00000000	0.00000000	-1.09706600	4	0.08312000	-0.13884700	-1.13869200

Table S3. Cartesian coordinates and energy (in au) for low-lying isomeric structures of $Be_2B_8^{2+}$ complex in singlet and triplet spin states at the B3LYP/def2-TZVP level of theory

3S-1		-227.435447270		**3T**		-227.39350083	
2 1				2 3			
5	1.76396500	-1.13757900	-0.00018500	5	-1.85434700	0.76729700	0.00000000
4	-4.56520900	-0.49263600	-0.00036500	5	-1.85434700	-0.76729700	0.00000000
5	0.19743500	-0.87003700	0.00015800	5	-0.76719900	-1.85038100	0.00000000
5	-1.76396300	1.13757600	-0.00002100	5	0.76719900	-1.85038100	0.00000000
5	2.88215300	-0.10329500	0.00000800	5	1.85434700	-0.76729700	0.00000000
5	-2.88214900	0.10329300	-0.00013700	5	1.85434700	0.76729700	0.00000000
5	-1.34816300	-0.50210900	0.00032400	5	0.76719900	1.85038100	0.00000000
5	-0.19743300	0.87005000	0.00018700	5	-0.76719900	1.85038100	0.00000000
5	1.34815800	0.50208600	0.00001100	4	0.00000000	0.00000000	1.09706600
4	4.56520600	0.49265500	-0.00006600	4	0.00000000	0.00000000	-1.09706600

3S-2		-227.420522569		**3T-1**		-227.392141158	
2 1				2 3			
5	1.37822700	-1.41242300	-0.16742200	5	0.06002500	-0.92076500	0.00000000
4	-0.05046500	-0.00064700	1.38160400	5	0.00000000	0.85871600	0.00000000
5	0.25864200	0.00011000	-0.48420600	5	2.78741200	0.73227600	0.00000000
5	-0.10906200	1.75176700	0.06423000	5	1.40851600	1.59468100	0.00000000
5	2.02912500	-0.00012400	-0.22567200	5	-1.39456200	0.05019100	0.00000000
5	-1.31548300	0.79954100	0.22031000	5	1.47480900	-0.09476200	0.00000000
5	-1.31588900	-0.79935700	0.22006800	4	-3.19953400	-2.39362400	0.00000000
5	1.37848100	1.41230100	-0.16741800	5	-1.34123600	-1.63383600	0.00000000
5	-0.10941500	-1.75154600	0.06385200	4	2.93976400	2.57251600	0.00000000
4	-2.69281800	0.00031100	-0.78628100	5	-2.78714700	-0.72961600	0.00000000

3S-3		-227.414570775		**3T-2**		-227.386768410	
2 1				2 3			
5	-1.42359100	0.67782700	-0.00005500	5	2.03334600	0.78495100	-0.06891200
4	4.57339800	0.12935800	0.00041800	5	-2.01781900	-0.00163300	0.01361200
5	-0.00001200	1.33114300	-0.00011400	5	2.03423700	-0.78329100	-0.06912800
5	0.00000800	-0.50785100	-0.00008000	5	-0.76243200	-0.99885800	-0.02857900
5	-4.57338600	0.12937800	0.00010800	4	0.66769600	0.00000300	1.23344700
5	-1.53642200	-0.99904600	-0.00014400	5	0.69892100	-1.57908400	-0.01281200
5	-2.82395300	-0.19394600	0.00006200	5	0.69720100	1.57934600	-0.01281000
5	1.53643500	-0.99903700	-0.00021800	4	-3.84476900	0.00118900	-0.03033600
5	1.42357200	0.67783500	-0.00000700	5	0.62165700	0.00020800	-0.75538900
4	2.82395400	-0.19391400	0.00013700	5	-0.76345300	0.99740800	-0.02847200

3S-4   -227.409819622

2 1
4   -3.46898300   -0.74047100   -0.34567800
5   2.04565400   0.80608800   -0.30453500
5   -1.89407200   -0.07875000   0.04053500
4   -1.27579100   1.64146400   -0.49509600
5   0.97387800   -1.61633200   -0.20398700
5   0.61525500   1.48439500   -0.02031500
5   -0.51952000   -1.03562600   0.12815900
5   2.25037900   -0.72904300   -0.27985100
5   -0.60743400   0.54067500   0.70190400
5   0.93168100   -0.09220100   0.61071100

3S-5   -227.400269973

2 1
4   -3.06398200   -0.00076300   -0.17221900
5   1.26844400   -1.40296500   -0.15852300
5   -1.41608700   0.79497400   0.16472200
5   1.75262700   0.00021400   -0.68418700
5   -0.00334700   0.00021100   -0.17497200
5   -0.21655600   -1.79991700   0.02815100
5   -1.41582100   -0.79451900   0.16523200
5   1.26838500   1.40299600   -0.15788500
5   -0.21664800   1.80023900   0.02827900
4   1.78773700   -0.00077800   1.15869900

3T-3   -227.385523815

2 3
4   3.52671100   1.86716400   0.00001000
5   -0.68585600   -1.05633800   -0.00005100
5   2.41156600   0.44786700   -0.00047400
5   -2.12090300   -0.33430100   -0.00000600
5   0.75215400   0.04060100   0.00019700
5   0.73607900   -1.73964500   -0.00004500
5   2.11183600   -1.05866700   0.00022700
4   -3.78992100   0.30930700   -0.00033900
5   -2.22062400   1.27312800   0.00016100
5   -0.77368500   0.68617800   0.00025500

3T-4   -227.384869772

2 3
5   0.35109400   -0.93821600   -0.00033100
4   -4.48048200   -0.39101400   0.00068000
5   -1.59375400   1.14066000   -0.00015100
5   -0.06497500   0.76468300   -0.00047900
5   -1.22986200   -0.50943700   -0.00026800
5   1.54272700   0.36902400   -0.00018900
5   -2.73588500   0.07088900   0.00043200
5   3.03481900   -0.38549400   0.00024600
4   3.01927600   1.44560800   0.00008300
5   1.86480000   -1.35578500   0.00013000

Table S3. Complete reference 73.

73   M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision B.01, Gaussian Inc., Wallingford CT, 2009