Supplementary Information for

Density Functional Theory Studies of Boron Clusters with Exotic Properties in Bonding, Aromaticity and Reactivity

Dongbo Zhao,[1] Xin He,[2] Meng Li,[2] Bin Wang,[2] Chunna Guo,[2] Chunying Rong,[2] Pratim K. Chattaraj,[3] and Shubin Liu[4,5]

[1] *Institute of Biomedical Research, Yunnan University, Chenggong District, Kunming 650500, Yunnan, P.R. China.*
E-mail: *dongbo@ynu.edu.cn*
[2] *Key Laboratory of Chemical Biology and Traditional Chinese Medicine Research (Ministry of Education of China), Hunan Normal University, Changsha, Hunan 410081, P.R. China*
E-mail: *rongchunying@aliyun.com*
[3] *Department of Chemistry, Indian Institute of Technology, Kharagpur 721302, India.* E-mail*:* pkc@chem.iitkgp.ac.in
[4]*Research Computing Center, University of North Carolina, Chapel Hill, North Carolina 27599-3420, USA.* E-mail*:* shubin@email.unc.edu
[5] *Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina, 27599-3290, USA*

1. Table S1, Cartesian coordinates of the 6 isomers of B_4 cluster
2. Figure S1, ELF isosurfaces for the 6 isomers

Table S1. Cartesian coordinates for isomers **1** to **6**

isomer **1**			
B	0.00000000	-1.19554720	-0.00000219
B	0.00000000	0.00000000	0.94309635
B	-0.00000000	-0.00000000	-0.94309197
B	0.00000000	1.19554720	-0.00000219
isomer **2**			
B	0.00000000	1.08609008	-0.00000000
B	1.08609008	-0.00000000	-0.00000000
B	-1.08609008	0.00000000	-0.00000000
B	-0.00000000	-1.08609008	-0.00000000
isomer **3**			
B	-0.00000000	-0.00000000	1.96655514
B	-0.00000000	-0.00000000	0.25876302
B	0.00000000	0.75460105	-1.11265908
B	-0.00000000	-0.75460105	-1.11265908
isomer **4**			
B	-0.59159804	-2.13970015	0.00000000
B	-0.62615304	-0.54919604	0.00000000
B	1.21775109	1.85641413	0.00000000
B	0.00000000	0.83248206	0.00000000
isomer **5**			
B	0.00000000	0.00000000	0.74354905
B	0.00000000	0.00000000	2.31105217
B	0.00000000	0.00000000	-0.74354905
B	0.00000000	0.00000000	-2.31105217
isomer **6**			
B	0.00000000	0.00000000	2.28372133
B	0.00000000	0.00000000	0.83938412
B	0.00000000	0.00000000	-2.28372133
B	0.00000000	0.00000000	-0.83938412

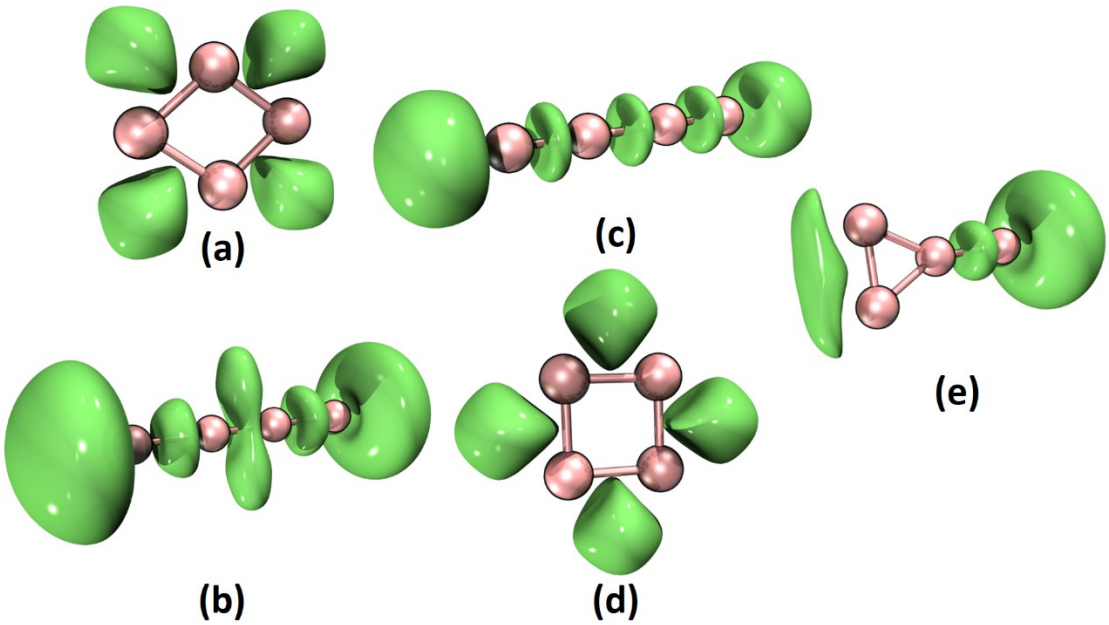

Figure S1. ELF diagrams of (a) rhombus isomer **1**, (b) linear isomer **5**, (c) linear isomer **6**, (d) square isomer **2**, and (e) capped triangle isomer **3**. Isovalue = 0.9 au.