Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

A theoretical approach to the role of different types of electron in planar elongated boron clusters

Long Van Duong[a], Dang Thi Tuyet Mai[b], My Phuong Pham-Ho[a], Minh Tho Nguyen[b,*]

[a]*Institute for Computational Science and Technology (ICST), Quang Trung Software City Ho Chi Minh, Vietnam*

[b]*Department of Chemistry, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium*

Email: minh.nguyen@kuleuven.be

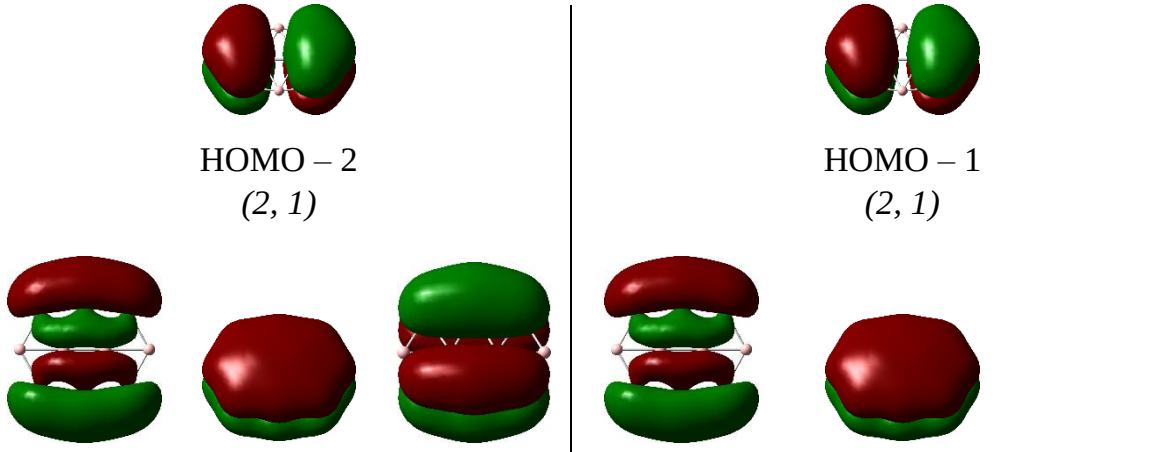
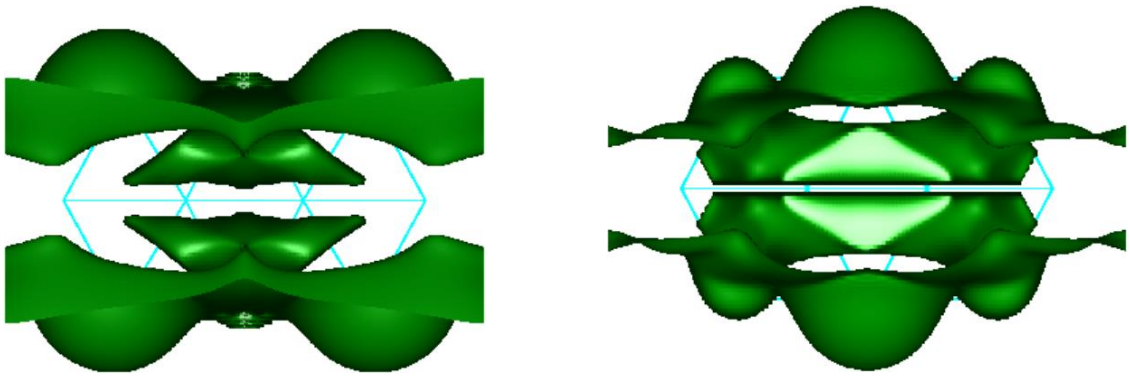
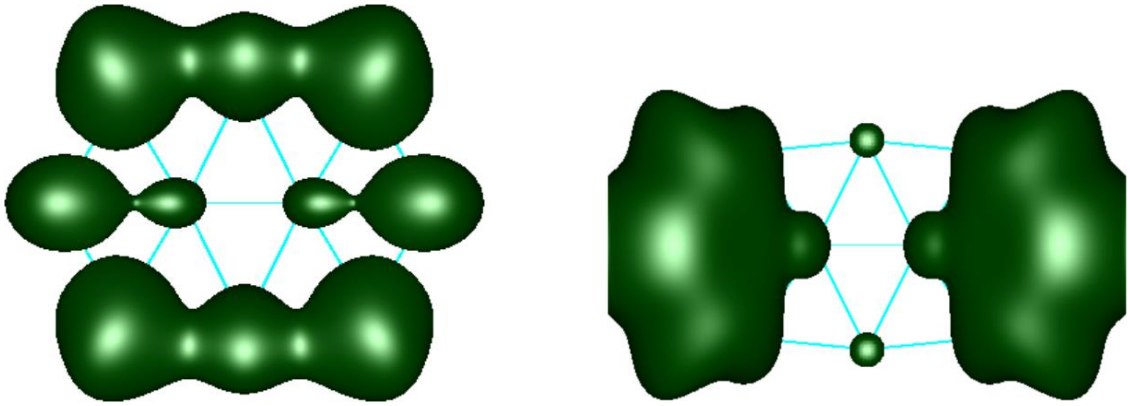


Figure S1. The separated delocalized MOs of B_{10} D_{2h} and B_{10}^{2+} D_{2h} into three catalogue: σ-MOs, π_1-MOs, and π_2-MOs.



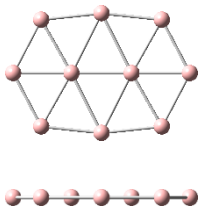
a) ELF(σ_loca) c) ELF(σ_loca)



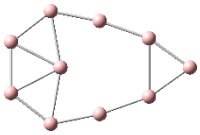
b) ELF_{π} d) ELF_{π}

B_{10} D_{2h} B_{10}^{2+} D_{2h}

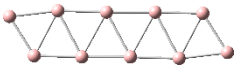
Figure S2. ELF(σ_delo) and ELF_{π} of B_{10} D_{2h} and B_{10}^{2+} D_{2h}.



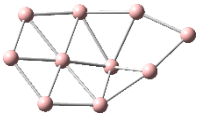
B10.dia.1 (D_{2h} ^1A_g)
0.00 {0.00}
[0.00]



B10.dia.2 (C_{2v} $^1A_1$)
13.28 {9.57}
[9.90]



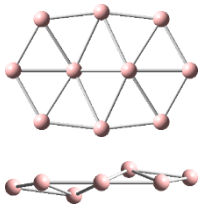
B10.dia.4 (C_{2h} ^3B_u)
24.66 {26.84}
[37.28]



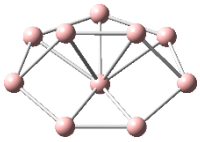
B10.dia.5 (C_s $^1A'$)
34.19 {32.83}
[33.63]

B10.dia.3 (C_{2h} ^3A_u)
22.92 {23.35}
[35.83]

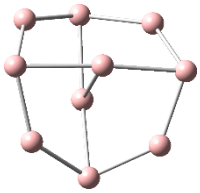
B10.dia.6 (C_{2h} ^1A_g)
35.85 {31.65}
[31.63]



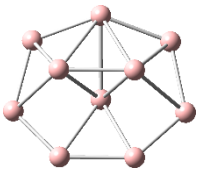
B10.n.1 (C_{2h} ^1A_g)
0.00 {0.00}
[0.00]



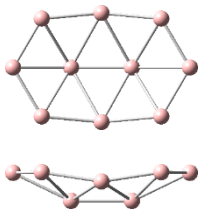
B10.n.2 (C_s $^1A'$)
10.14 {8.44}
[12.03]



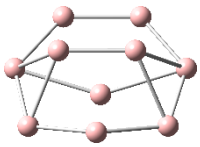
B10.n.3 (D_{2d} $^1A_1$)
20.93 {25.88}
[31.52]



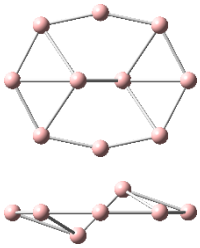
B10.n.4 (C_s $^3A''$)
32.65 {31.07}
[43.33]



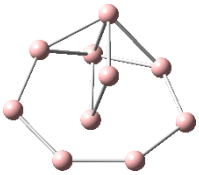
B10.dic.1 (C_{2v} $^1A_1$)
0.00 {0.00}
[0.00]



B10.dic.2 (Cs $^1A'$)
5.41 {5.23}
[4.38]



B10.dic.3 (C_{2h} ^1A_g)
11.49 {8.51}
[12.67]



B10.dic.4 (C_2 ^1A)
12.26 {11.18}
[67.59]

Figure S3. Global energy minima structures of B_{10} in dianionic, anionic, neutral, cationic and dication states. Relative energies (E, kcal/mol) are obtained from PBE0/6-311+G(d) +ZPE, TPSSh/6-311+G(d)+ZPE, (in curly brackets) and CCSD(T)/CBS_{D-T} (in square brackets) calculations.

Cartesian Coordinates and Total Energies of the Optimized Structures Condidered

B10.dia.1

TPSSh/6-311+G(d): E = -248.38270 Hartree; ZPE = 0.03885 Hartree

PBE0/6-311+G(d): E = -247.99663 Hartree; ZPE = 0.03958 Hartree

5	-0.000000000	1.442169000	1.624637000
5	0.000000000	-0.000000000	-0.811570000
5	0.000000000	-1.615501000	-0.000000000
5	0.000000000	-0.000000000	-2.379169000
5	-0.000000000	-0.000000000	2.379169000
5	-0.000000000	-1.442169000	-1.624637000
5	-0.000000000	-1.442169000	1.624637000
5	0.000000000	1.442169000	-1.624637000
5	0.000000000	1.615501000	-0.000000000
5	-0.000000000	-0.000000000	0.811570000

B10.dia.2

TPSSh/6-311+G(d): E = -248.367440872 Hartree; ZPE = 0.037974 Hartree

PBE0/6-311+G(d): E = -247.974083985 Hartree; ZPE = 0.038200 Hartree

5	0.000000000	1.437832000	0.387787000
5	0.000000000	1.740223000	-1.124624000
5	0.000000000	0.000000000	-0.822803000
5	0.000000000	0.899485000	1.912946000
5	0.000000000	-0.788215000	-2.354275000
5	0.000000000	-1.437832000	0.387787000
5	0.000000000	0.788215000	-2.354275000
5	0.000000000	0.000000000	3.179134000
5	0.000000000	-0.899485000	1.912946000
5	0.000000000	-1.740223000	-1.124624000

B10.dia.3

TPSSh/6-311+G(d): E = -248.345495610 Hartree; ZPE = 0.036574 Hartree

PBE0/6-311+G(d): E = -247.957873701 Hartree; ZPE = 0.037354 Hartree

5	-0.000000000	1.642935000	1.411129000
5	-0.256685000	-0.785025000	-0.000000000

5	-0.000000000	-0.000000000	-1.540849000
5	0.027164000	-2.410000000	-0.000000000
5	-0.027164000	2.410000000	-0.000000000
5	-0.000000000	-1.642935000	-1.411129000
5	-0.000000000	1.642935000	-1.411129000
5	-0.000000000	-1.642935000	1.411129000
5	0.000000000	-0.000000000	1.540849000
5	0.256685000	0.785025000	-0.000000000

B10.dia.4

TPSSh/6-311+G(d): E = -248.339932037 Hartree; ZPE = 0.037046 Hartree

PBE0/6-311+G(d): E = -247.947533959 Hartree; ZPE = 0.037754 Hartree

5	1.436048000	0.085171000	0.000000000
5	-2.837573000	0.691807000	0.000000000
5	1.436048000	-1.647238000	0.000000000
5	-1.436048000	1.647238000	0.000000000
5	-0.008310000	0.845643000	0.000000000
5	-1.436048000	-0.085171000	0.000000000
5	-2.963677000	2.232527000	0.000000000
5	2.963677000	-2.232527000	0.000000000
5	0.008310000	-0.845643000	0.000000000
5	2.837573000	-0.691807000	0.000000000

B10.dia.5

TPSSh/6-311+G(d): E = -248.330377591 Hartree; ZPE = 0.038442 Hartree

PBE0/6-311+G(d): E = -247.941177027 Hartree; ZPE = 0.038616 Hartree

5	0.273355000	0.023641000	1.468203000
5	-0.554362000	2.301660000	0.000000000
5	-0.229618000	1.588453000	1.405226000
5	0.273355000	0.023641000	-1.468203000
5	-0.229618000	-1.487280000	-0.941406000
5	-0.229618000	1.588453000	-1.405226000
5	-0.229618000	-1.487280000	0.941406000
5	0.991890000	-0.603789000	0.000000000
5	-0.178143000	-2.767447000	0.000000000
5	0.112378000	0.819950000	0.000000000

B10.dia.6

TPSSh/6-311+G(d): E = -248.332253431 Hartree; ZPE = 0.037513 Hartree

PBE0/6-311+G(d): E = -247.937754617 Hartree; ZPE = 0.037832 Hartree

5	1.438602000	0.115497000	0.000000000
5	-2.819808000	0.737836000	0.000000000
5	1.438602000	-1.687509000	0.000000000
5	-1.438602000	1.687509000	0.000000000
5	-0.009615000	0.838550000	0.000000000
5	-1.438602000	-0.115497000	0.000000000
5	-2.915800000	2.267799000	0.000000000
5	2.915800000	-2.267799000	0.000000000
5	0.009615000	-0.838550000	0.000000000
5	2.819808000	-0.737836000	0.000000000

B10.n.1

TPSSh/6-311+G(d): E = -248.35126 Hartree; ZPE = 0.040916 Hartree

PBE0/6-311+G(d): E = -247.959277695 Hartree; ZPE = 0.037832 Hartree

5	0.000000000	1.608521000	1.382679000
5	0.000000000	0.000000000	1.570862000
5	0.000000000	0.000000000	-1.570862000
5	0.000000000	1.608521000	-1.382679000
5	-0.124735000	2.379345000	0.000000000
5	-0.340884000	0.738646000	0.000000000
5	0.340884000	-0.738646000	0.000000000
5	0.000000000	-1.608521000	-1.382679000
5	0.000000000	-1.608521000	1.382679000
5	0.124735000	-2.379345000	0.000000000

B10.n.2

TPSSh/6-311+G(d): E = -248.335579282 Hartree; ZPE = 0.037927 Hartree

PBE0/6-311+G(d): E = -247.940768881 Hartree; ZPE = 0.038566 Hartree

5	0.379509000	-0.154786000	1.896922000
5	-0.669126000	0.924887000	1.464898000
5	0.379509000	-0.154786000	-1.896922000
5	-0.669126000	0.924887000	-1.464898000
5	-1.173762000	1.245889000	0.000000000

5	1.355301000	-0.767535000	0.784208000
5	0.380647000	0.465129000	0.000000000
5	1.355301000	-0.767535000	-0.784208000
5	-0.669126000	-0.858076000	-0.772855000
5	-0.669126000	-0.858076000	0.772855000

B10.n3

TPSSh/6-311+G(d): E = -248.306986335 Hartree; ZPE = 0.037120 Hartree

PBE0/6-311+G(d): E = -247.910039997 Hartree; ZPE = 0.037784 Hartree

5	1.284962000	1.284962000	0.000000000
5	1.711255000	0.000000000	0.751768000
5	-1.711255000	0.000000000	0.751768000
5	-1.284962000	-1.284962000	0.000000000
5	0.000000000	-1.711255000	-0.751768000
5	0.000000000	1.711255000	-0.751768000
5	0.000000000	0.000000000	0.923365000
5	-1.284962000	1.284962000	0.000000000
5	1.284962000	-1.284962000	0.000000000
5	0.000000000	0.000000000	-0.923365000

B10.n.4

TPSSh/6-311+G(d): E = -248.298836361 Hartree; ZPE = 0.037240 Hartree

PBE0/6-311+G(d): E = -247.904351817 Hartree; ZPE = 0.038020 Hartree

5	0.429589000	0.346709000	1.834731000
5	-1.131687000	0.322588000	1.473483000
5	0.429589000	0.346709000	-1.834731000
5	-1.131687000	0.322588000	-1.473483000
5	-1.553543000	-0.140684000	0.000000000
5	1.548262000	0.003178000	0.800311000
5	0.043384000	0.700271000	0.000000000
5	1.548262000	0.003178000	-0.800311000
5	-0.091084000	-0.952269000	-0.807658000
5	-0.091084000	-0.952269000	0.807658000

B10.dic.1

TPSSh/6-311+G(d): E = -247.553988661 Hartree; ZPE = 0.037644 Hartree

PBE0/6-311+G(d): E = -247.155479503 Hartree; ZPE = 0.038371 Hartree

5	0.000000000	2.415968000	-0.190321000
5	1.343327000	1.632978000	-0.207658000
5	-1.343327000	1.632978000	-0.207658000
5	0.000000000	0.832242000	0.564417000
5	0.000000000	-0.832242000	0.564417000
5	0.000000000	-2.415968000	-0.190321000
5	-1.343327000	-1.632978000	-0.207658000
5	-1.496576000	0.000000000	0.041220000
5	1.496576000	0.000000000	0.041220000
5	1.343327000	-1.632978000	-0.207658000

B10.dic.2

TPSSh/6-311+G(d): E = -247.545308916 Hartree; ZPE = 0.037296 Hartree

PBE0/6-311+G(d): E = -247.146601281 Hartree; ZPE = 0.038118 Hartree

5	0.469609000	0.279099000	1.766054000
5	-1.072083000	0.408940000	1.438936000
5	-1.647404000	0.014022000	0.000000000
5	-0.302751000	-1.015777000	0.792296000
5	0.105867000	0.670220000	0.000000000
5	-1.072083000	0.408940000	-1.438936000
5	-0.302751000	-1.015777000	-0.792296000
5	1.675994000	-0.014383000	-0.797356000
5	0.469609000	0.279099000	-1.766054000
5	1.675994000	-0.014383000	0.797356000

B10.dic.3

TPSSh/6-311+G(d): E = -247.538941230 Hartree; ZPE = 0.036159 Hartree

PBE0/6-311+G(d): E = -247.137172138 Hartree; ZPE = 0.036841 Hartree

5	0.000000000	0.000000000	1.742328000
5	-0.005894000	2.268685000	0.000000000
5	0.000000000	1.528315000	1.416886000
5	-0.595957000	0.578389000	0.000000000
5	0.000000000	1.528315000	-1.416886000
5	0.000000000	-1.528315000	1.416886000
5	0.000000000	0.000000000	-1.742328000
5	0.000000000	-1.528315000	-1.416886000

5	0.005894000	-2.268685000	0.000000000
5	0.595957000	-0.578389000	0.000000000

B10.dic.4

TPSSh/6-311+G(d): E = -247.534657065 Hartree; ZPE = 0.036121 Hartree

PBE0/6-311+G(d): E = -247.134553229 Hartree; ZPE = 0.036976 Hartree

5	-0.898373000	1.003913000	-0.890019000
5	-0.588583000	-0.568595000	-1.519666000
5	0.651144000	0.609829000	0.110885000
5	0.588583000	0.568595000	-1.519666000
5	0.898373000	-1.003913000	-0.890019000
5	1.414518000	-1.218423000	0.578829000
5	0.651144000	-0.431962000	1.719971000
5	-0.651144000	0.431962000	1.719971000
5	-0.651144000	-0.609829000	0.110885000
5	-1.414518000	1.218423000	0.578829000