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

SUPPLEMENTARY INFORMATION

$Y©B_8C_4$ Cluster: A Boron-Carbon Molecular Wheel with Dodeca-coordination Number in Plane

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Supplementary Information

Table S1. Cartesian coordinates for the D_{4h} ($^2B_{1u}$) global-minimum (GM) structure of $Y©B_8C_4$ cluster at PBE0/B,C/6-311+G*/Y/Stuttgart'97 level.

Figure S1. Alternative optimized Low-lying isomers of $Y©B_8C_4$ cluster. All energies are in eV. The relative energies are shown at the single-point CCSD(T)/Y/Stuttgart'97/B,C/6-311+G*//PBE0/Y/Stuttgart'97/B,C/6-311+G* level (for top ten), at PBE0/Y/Stuttgart'97/B,C/6-311+G* level (in square brackets), and at B3LYP/Y/Stuttgart'97/B,C/6-311+G* level (in curly brackets), respectively. The relative energies at both PBE0 and B3LYP levels are corrected with the zero-point energies (ZPEs).

Figure S2. The top five isomers of (a) $Y©B_8C_4^+$ and (b) $Y©B_8C_4^-$ clusters at PBE0/Y/Stuttgart'97/B,C/6-311+G* level. The relative energies (in eV) are corrected with ZPEs.

Figure S3. Calculated bond distances (in Å) at PBE0/Y/Stuttgart'97/B,C/6-311+G* level for (a) D_{4h} ($^2B_{1u}$) GM $Y©B_8C_4$ cluster, along with their (b) Wiberg bond indices (WBIs) and (c) natural atomic charges in |e| from the natural bond orbital (NBO) analyses at PBE0/Y/Stuttgart'97/B,C/6-311G* level.

Figure S4. Occupied canonical molecular orbitals (CMOs) of the D_{4h} ($^2B_{1u}$) GM $Y©B_8C_4$ cluster. (a) Twelve σ CMOs for two-center two-electron (2c-2e) B–C/B–B Lewis σ bonds in B_8C_4 ring. (b) Five delocalized σ CMOs in $Y©B_8C_4$. (c) Five delocalized π CMOs in $Y©B_8C_4$, the SOMO represents single occupation.

Figure S5. The CMOs energy diagram of delocalized σ/π frameworks in D_{4h} ($^2B_{1u}$) GM $Y©B_8C_4$ cluster.

Figure S6. The energy cycle of D_{4h} ($^2B_{1u}$) GM $Y©B_8C_4$ cluster, along with the isomerization energy of B_8C_4 ring, bond dissociation energy (BDE) and inherent interaction energy between the central Y and B_8C_4 ring (in kcal mol^{-1}).

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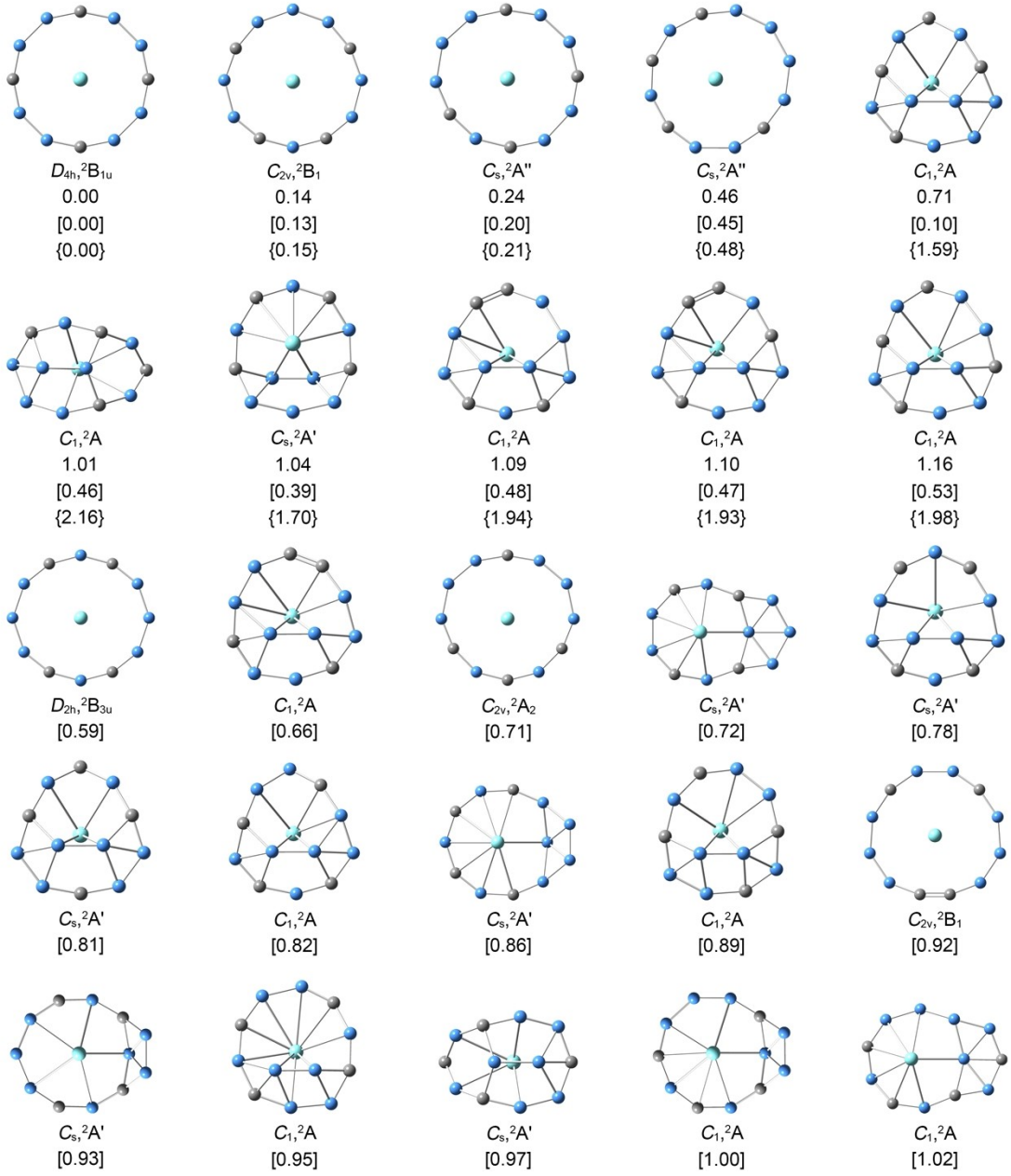

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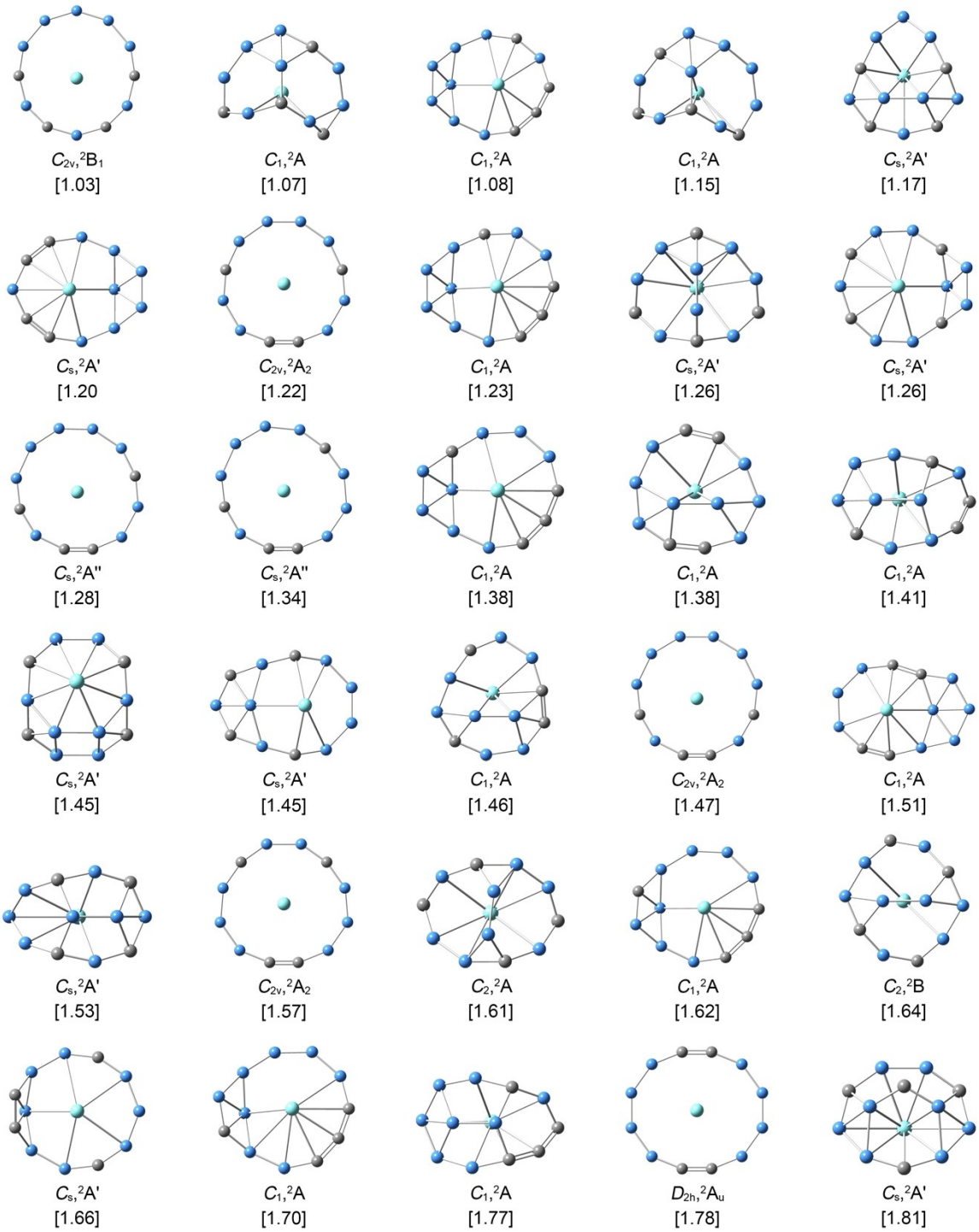
C_{2v},$^2B_1$
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C_1,^2A
[1.07]
C_1,^2A
[1.08]
C_1,^2A
[1.15]
C_s,$^2A'$
[1.17]
C_s,$^2A'$
[1.20
C_{2v},$^2A_2$
[1.22]
C_1,^2A
[1.23]
C_s,$^2A'$
[1.26]
C_s,$^2A'$
[1.26]
C_s,$^2A''$
[1.28]
C_s,$^2A''$
[1.34]
C_1,^2A
[1.38]
C_1,^2A
[1.38]
C_1,^2A
[1.41]
C_s,$^2A'$
[1.45]
C_s,$^2A'$
[1.45]
C_1,^2A
[1.46]
C_{2v},$^2A_2$
[1.47]
C_1,^2A
[1.51]
C_s,$^2A'$
[1.53]
C_{2v},$^2A_2$
[1.57]
C_2,^2A
[1.61]
C_1,^2A
[1.62]
C_2,^2B
[1.64]
C_s,$^2A'$
[1.66]
C_1,^2A
[1.70]
C_1,^2A
[1.77]
D_{2h},^2A_u
[1.78]
C_s,$^2A'$
[1.81]

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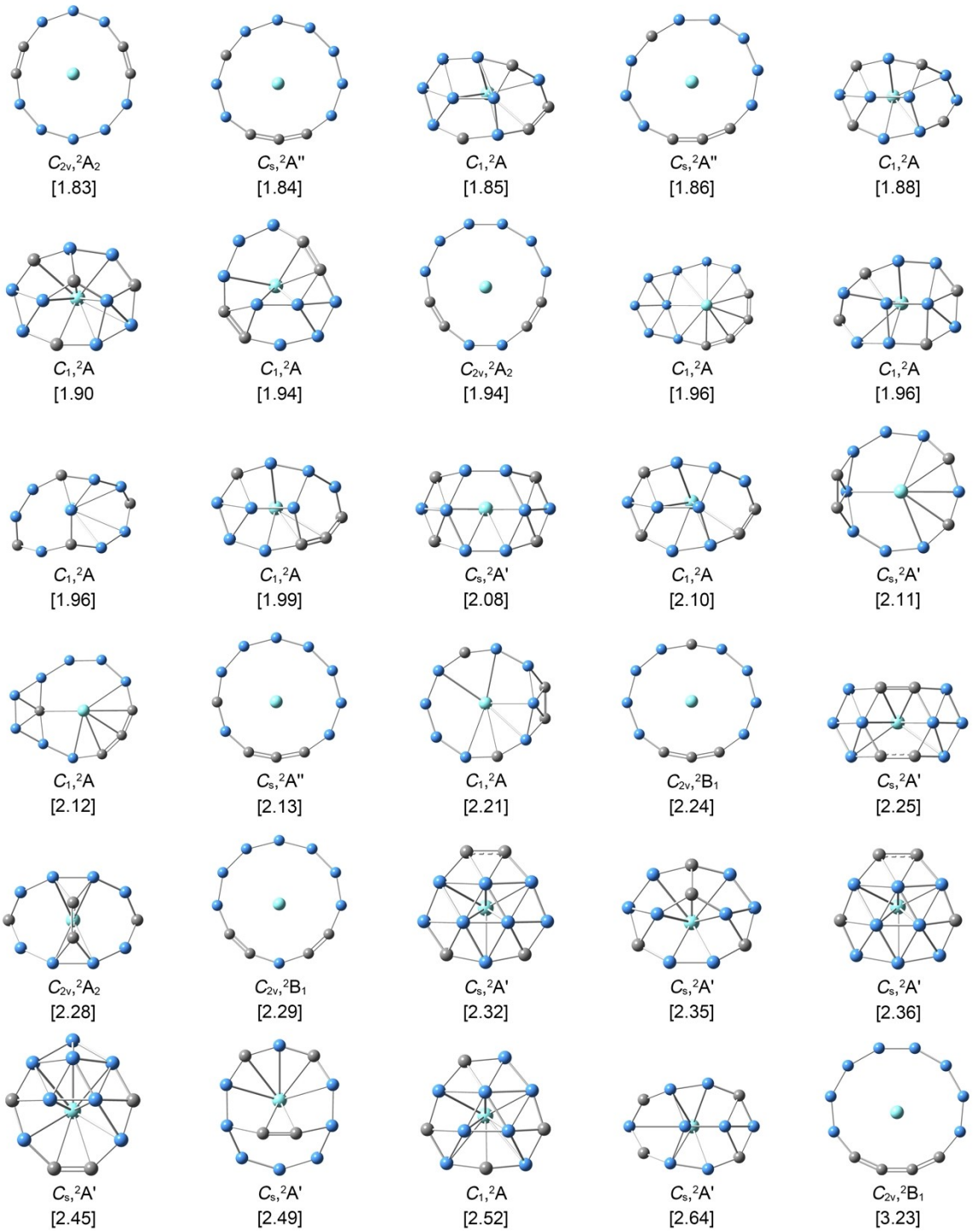
C_{2v},$^2A_2$ [1.83]
C_s,$^2A''$ [1.84]
C_1,^2A [1.85]
C_s,$^2A''$ [1.86]
C_1,^2A [1.88]
C_1,^2A [1.90
C_1,^2A [1.94]
C_{2v},$^2A_2$ [1.94]
C_1,^2A [1.96]
C_1,^2A [1.96]
C_1,^2A [1.96]
C_1,^2A [1.99]
C_s,$^2A'$ [2.08]
C_1,^2A [2.10]
C_s,$^2A'$ [2.11]
C_1,^2A [2.12]
C_s,$^2A''$ [2.13]
C_1,^2A [2.21]
C_{2v},$^2B_1$ [2.24]
C_s,$^2A'$ [2.25]
C_{2v},$^2A_2$ [2.28]
C_{2v},$^2B_1$ [2.29]
C_s,$^2A'$ [2.32]
C_s,$^2A'$ [2.35]
C_s,$^2A'$ [2.36]
C_s,$^2A'$ [2.45]
C_s,$^2A'$ [2.49]
C_1,^2A [2.52]
C_s,$^2A'$ [2.64]
C_{2v},$^2B_1$ [3.23]

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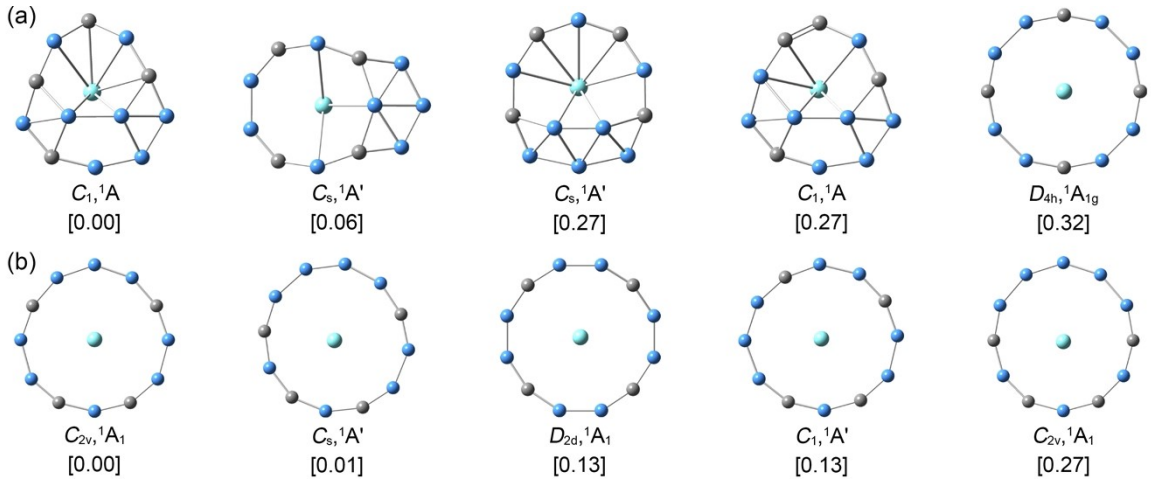

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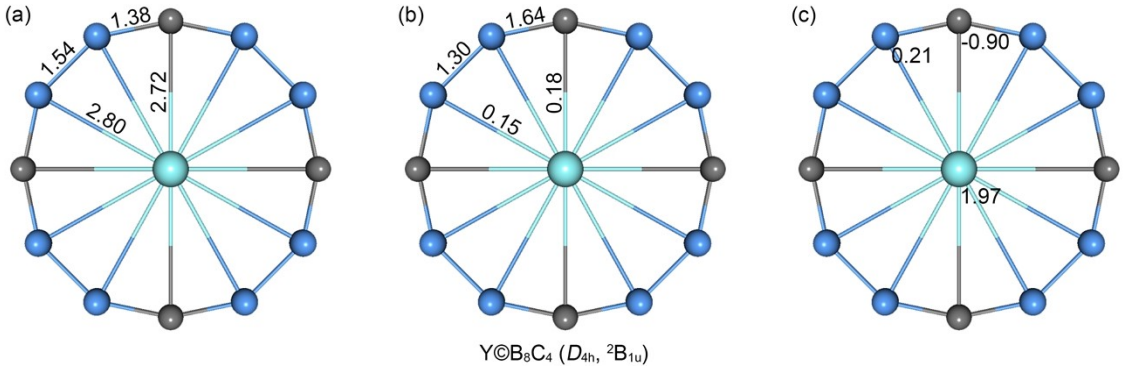

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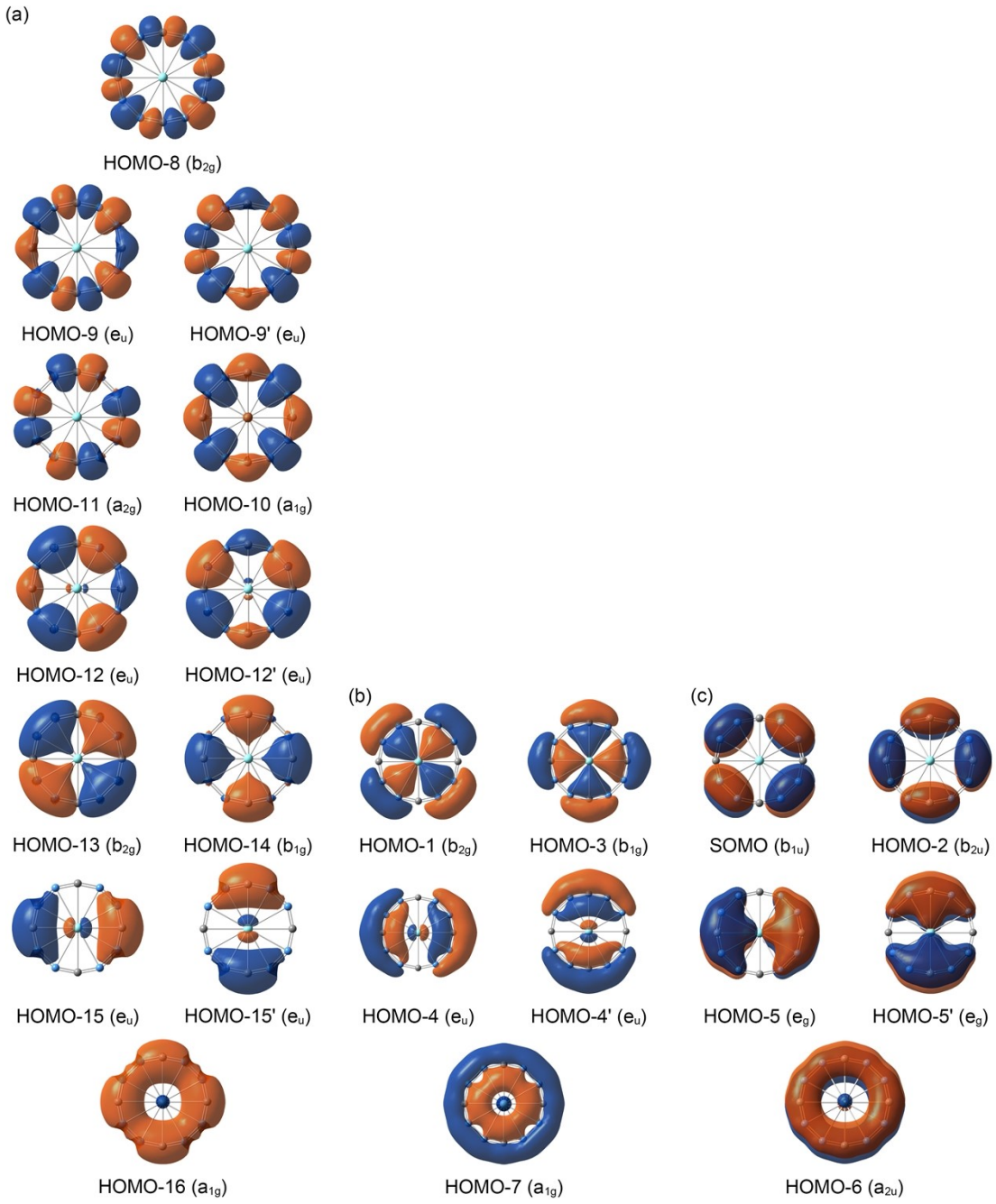

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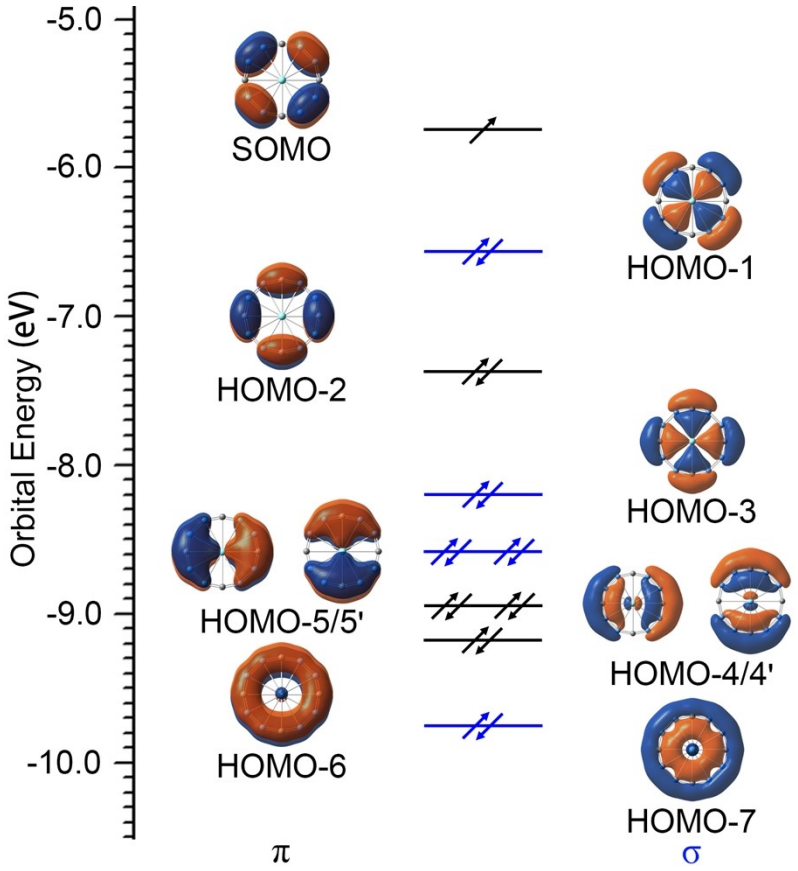

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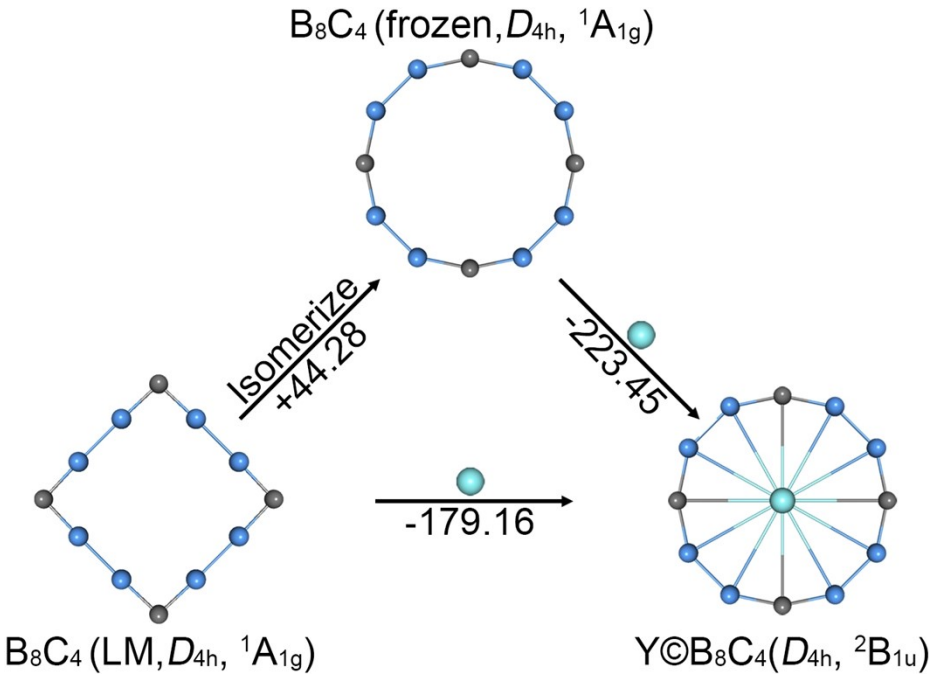

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Y©B_8C_4 GM (D_{4h}, $^2B_{1u}$)

C	0.00000000	2.71839600	0.00000000
C	0.00000000	-2.71839600	0.00000000
C	2.71839600	0.00000000	0.00000000
C	-2.71839600	0.00000000	0.00000000
B	2.44549100	1.35592000	0.00000000
B	1.35592000	2.44549100	0.00000000
B	-1.35592000	2.44549100	0.00000000
B	-2.44549100	1.35592000	0.00000000
B	-2.44549100	-1.35592000	0.00000000
B	-1.35592000	-2.44549100	0.00000000
B	1.35592000	-2.44549100	0.00000000
B	2.44549100	-1.35592000	0.00000000
Y	0.00000000	0.00000000	0.00000000