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SUPPORTING INFORMATION

Be₂B₆ and Be₂B₇⁺: two double aromatic inverse sandwich complexes with spin-triplet ground state

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SUPPORTING INFORMATION

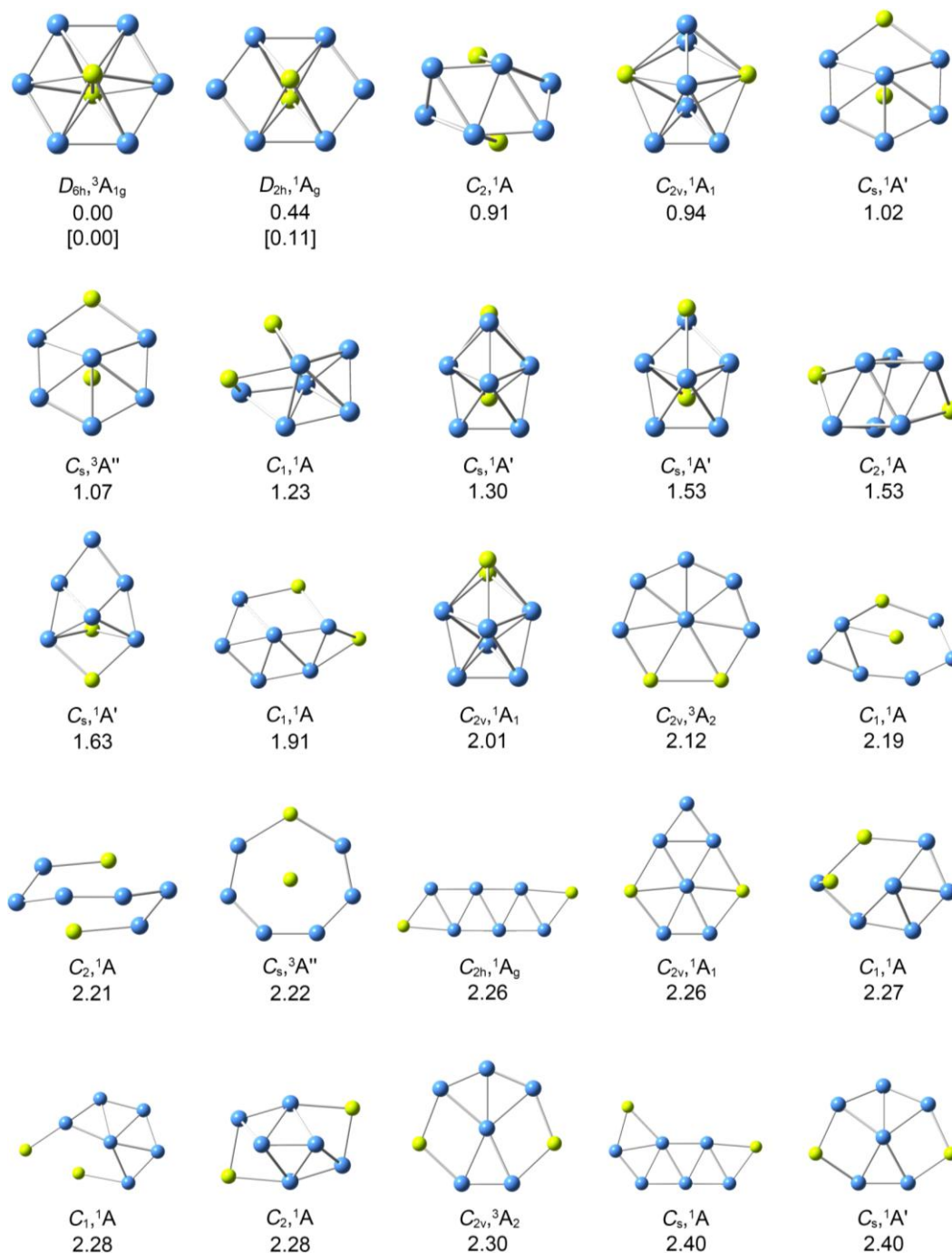
Table S1. Cartesian coordinates for global-minimum (GM) structures of (a) (*D*_{6h}, ³A_{1g}) Be₂B₆ and (b) (*D*_{7h}, ³A_{2'}) Be₂B₇⁺ clusters at the PBE0/6-311+G* level.

Figure S1. Alternative optimized structures of Be₂B₆ cluster at the PBE0/6-311+G* level. Relative energies are shown in eV at PBE0 level with corrections for zero-point energies (ZPEs), as well as for top two isomers (in square bracket) at the single-point CCSD(T)/6-311+G**//PBE0/6-311+G* level.

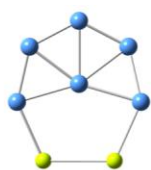
- Figure S2.** Alternative optimized structures of Be_2B_7^+ cluster at the PBE0/6-311+G* level. Relative energies are shown in eV at PBE0 level with corrections for zero-point energies (ZPEs), as well as for top two isomers (in square bracket) at the single-point CCSD(T)/6-311+G*/PBE0/6-311+G* level.
- Figure S3.** Canonical molecular orbitals (CMOs) of (D_{7h} , $^3A_2'$) Be_2B_7^+ . The CMOs are sorted to three subsets: (a) seven peripheral B–B σ single bonds; (b) globally delocalized 4σ framework; (c) globally delocalized 6π framework.
- Figure S4.** The adaptive natural density partitioning (AdNDP) bonding pattern of (D_{7h} , $^3A_2'$) Be_2B_7^+ cluster. Occupation numbers (ONs) are indicated.
- Figure S5.** Optimized structures of Be_2B_5^- cluster at the PBE0/6-311+G* level. Relative energies are shown in eV at the single-point CCSD(T)/6-311+G*/PBE0/6-311+G* and PBE0/6-311+G* (in square bracket) levels. The energies at the PBE0 level are corrected for zero-point energies (ZPEs).

Figure S1. Alternative optimized structures of Be_2B_6 cluster at the PBE0/6-311+G* level.

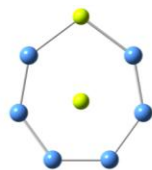
Relative energies are shown in eV at PBE0 level with corrections for zero-point energies (ZPEs), as well as for top two isomers (in square bracket) at the single-point CCSD(T)/6-311+G**/PBE0/6-311+G* level.



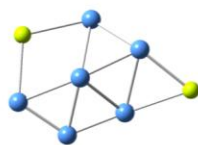
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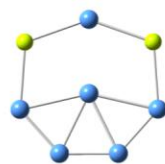
$C_{2v}, 1A$
2.41



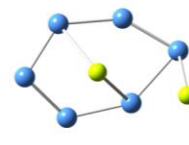
$C_{s}, 1A'$
2.41



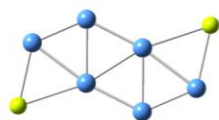
$C_{1}, 1A$
2.43



$C_{2v}, 1A_1$
2.48



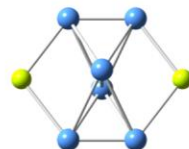
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$C_{2h}, 1A_g$
2.56



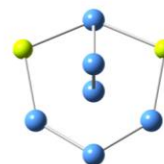
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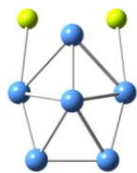
$D_{2h}, 1A_g$
2.74



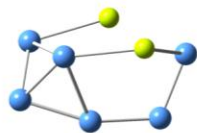
$C_{2v}, 1A_1$
2.76



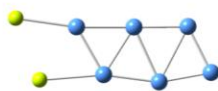
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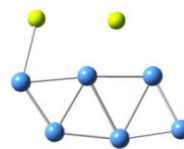
$C_{s}, 1A'$
2.87



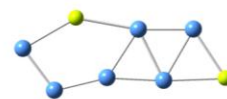
$C_{1}, 1A$
3.03



$C_{s}, 1A'$
3.03



$C_{1}, 1A$
3.06

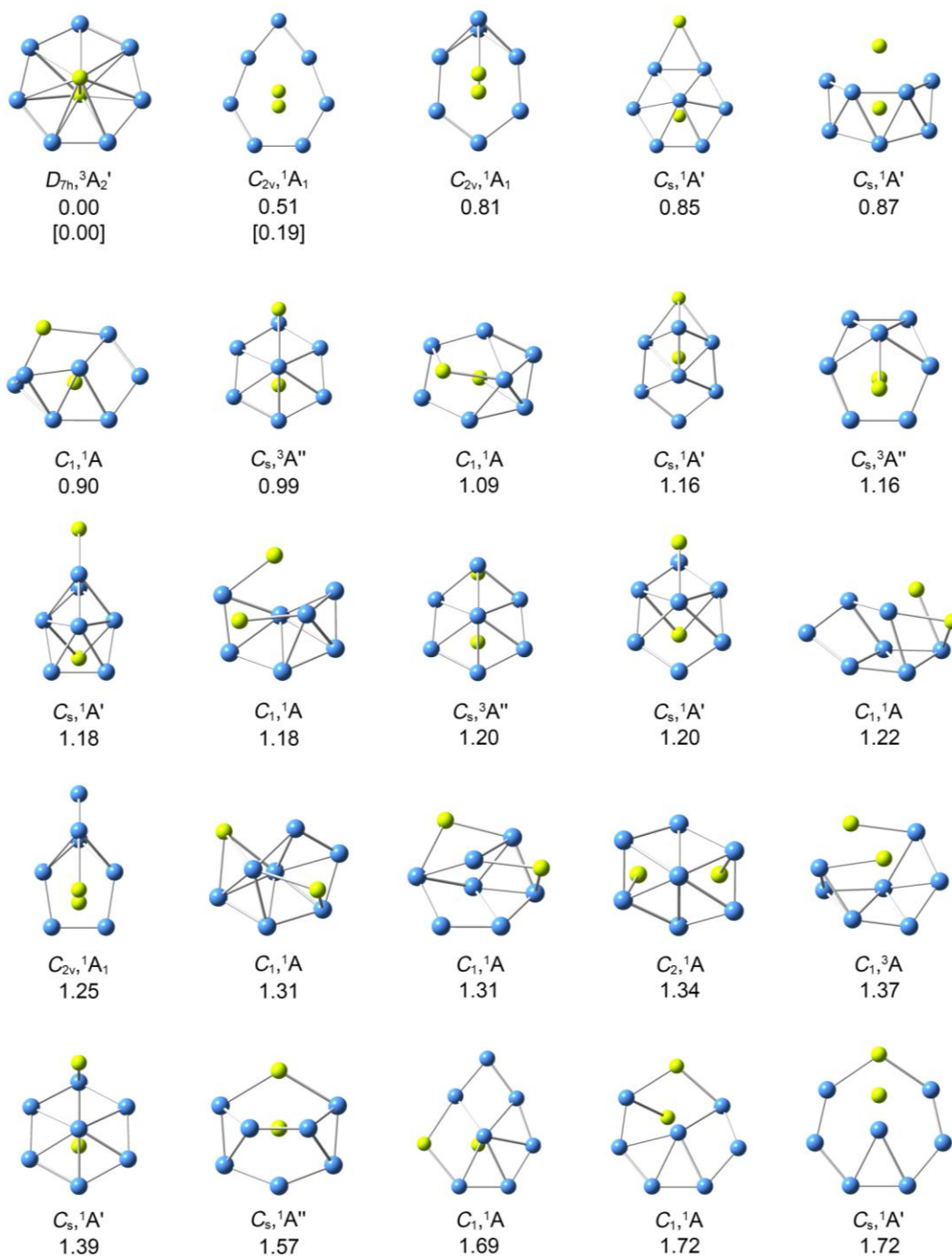


$C_{s}, 1A'$
3.25



$D_{2h}, 1A_{1g}$
5.81

Figure S2. Alternative optimized structures of Be_2B_7^+ cluster at the PBE0/6-311+G* level. Relative energies are shown in eV at PBE0 level with corrections for zero-point energies (ZPEs), as well as for top two isomers (in square bracket) at the single-point CCSD(T)/6-311+G**/PBE0/6-311+G* level.



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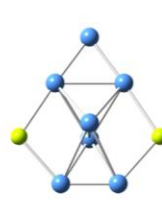
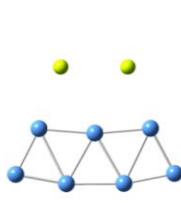
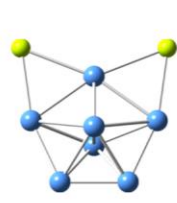
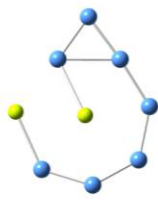
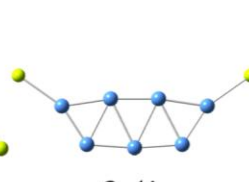
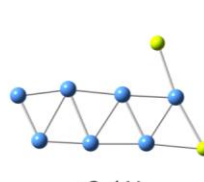
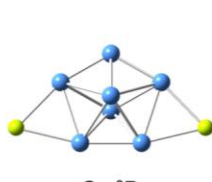
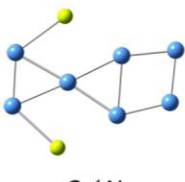
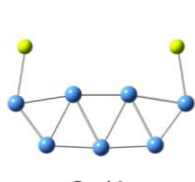
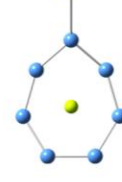
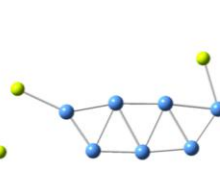
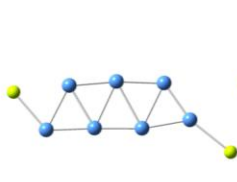
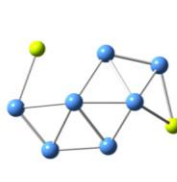
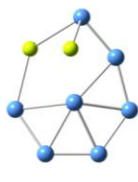
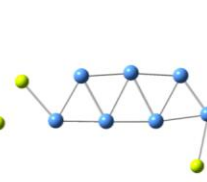
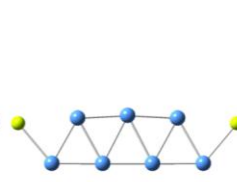
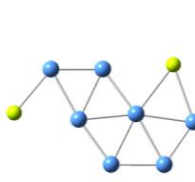
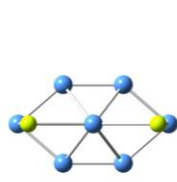
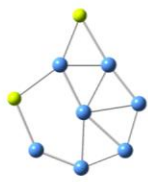
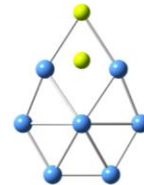
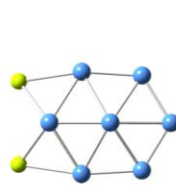
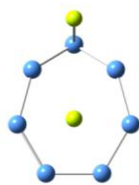
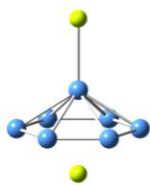
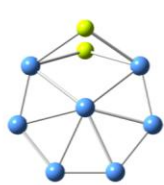


Figure S3. Canonical molecular orbitals (CMOs) of (D_{7h} , $^3A_2'$) Be_2B_7^+ . The CMOs are sorted to three subsets: (a) seven peripheral B–B σ single bonds; (b) globally delocalized 4σ framework; (c) globally delocalized 6π framework.

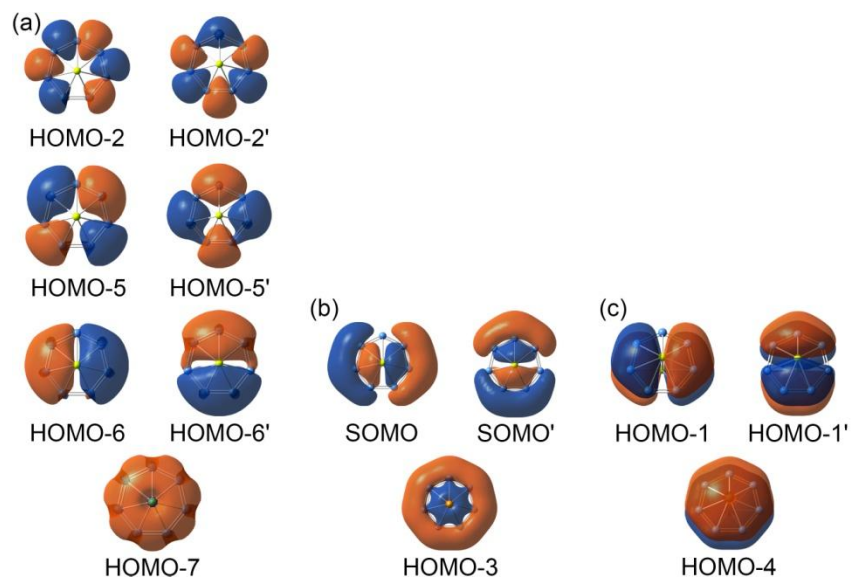


Figure S4. The adaptive natural density partitioning (AdNDP) bonding pattern of (D_{7h} , 3A_2) $Be_2B_7^+$ cluster. Occupation numbers (ONs) are indicated.

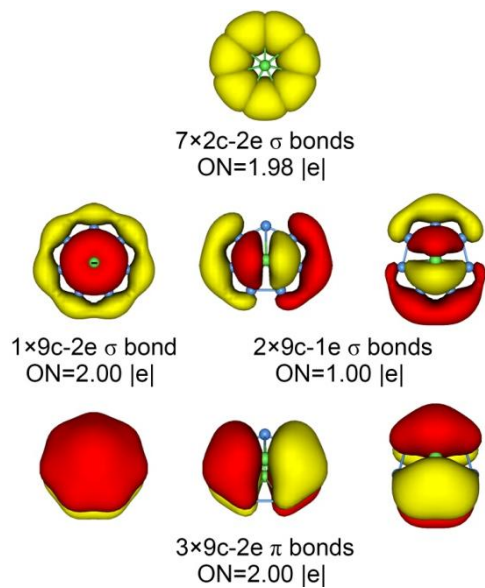


Figure S5. Optimized structures of Be_2B_5^- cluster at the PBE0/6-311+G* level. Relative energies are shown in eV at the single-point CCSD(T)/6-311+G**/PBE0/6-311+G* and PBE0/6-311+G* (in square bracket) levels. The energies at the PBE0 level are corrected for zero-point energies (ZPEs).

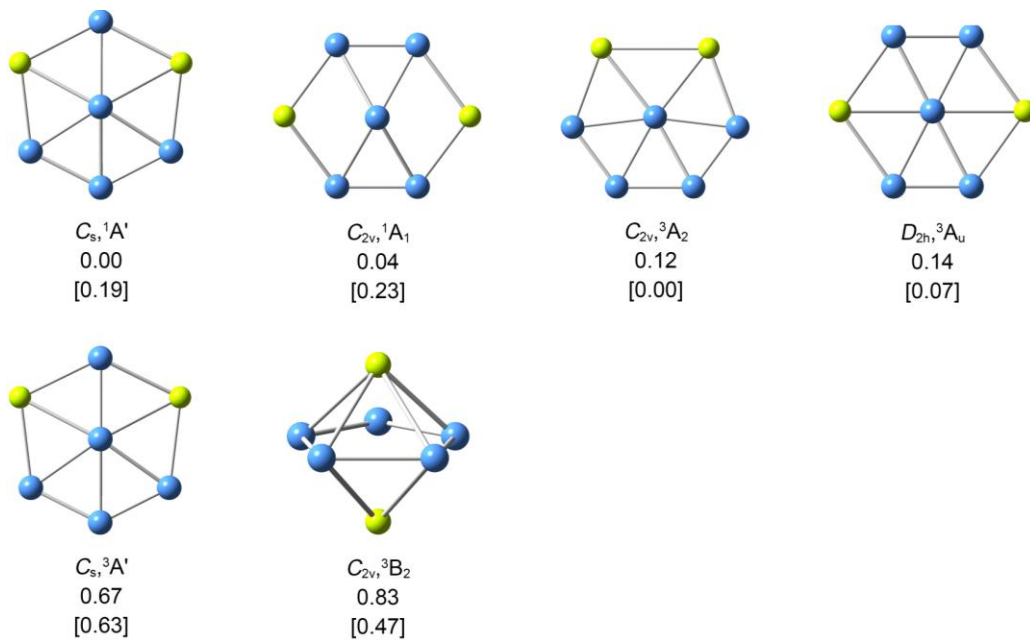


Table S1. Cartesian coordinates for global-minimum (GM) structures of (a) (D_{6h} , ${}^3A_{1g}$) Be_2B_6 and (b) (D_{7h} , ${}^3A_2'$) $Be_2B_7^+$ clusters at the PBE0/6-311+G* level.

(a) Be_2B_6 (D_{6h} , ${}^3A_{1g}$)

B	0.00000000	1.57221600	0.00000000
B	-1.36157900	0.78610800	0.00000000
B	-1.36157900	-0.78610800	0.00000000
B	0.00000000	-1.57221600	0.00000000
B	1.36157900	-0.78610800	0.00000000
B	1.36157900	0.78610800	0.00000000
Be	0.00000000	0.00000000	1.09717100
Be	0.00000000	0.00000000	-1.09717100

(b) $Be_2B_7^+$ (D_{7h} , ${}^3A_2'$)

B	0.00000000	1.77730400	-0.00000000
B	-0.77114331	-1.60129557	-0.00000000
B	-1.73274328	-0.39548735	-0.00000000
B	1.73274328	-0.39548735	-0.00000000
B	1.38955222	1.10813092	-0.00000000
B	-1.38955222	1.10813092	-0.00000000
B	0.77114331	-1.60129557	-0.00000000
Be	0.00000000	-0.00000000	1.06748000
Be	-0.00000000	-0.00000000	-1.06748000