SUPPLEMENTARY INFORMATION

Anchoring a bow-shaped boron single chain in binary Be$_6$B$_7^-$ cluster: hybrid octagonal ring, multifold π/σ aromaticity, and dual electronic transmutation

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Table S1   Cartesian coordinates for selected optimized structures of Be$_6$B$_7^-$ cluster at the PBE0/6-311+G(d) level. (a) Global-minimum (GM) C_{2v} ($^1A_1$) cluster. (b) Sandwich-type C_1 (^1A) structure. (c) Helix-type C_2 (^1A) structure.

Figure S1   Selected optimized sandwich- and helix-type isomeric structures of Be$_6$B$_7^-$ cluster at the PBE0/6-311+G(d) level along with their relative energies (in kcal mol^{-1}) above the GM structure, including zero-point energy (ZPE) corrections. Also presented are energetics data at the PBE0-D3/6-311+G(d) (in *italics*, with ZPE corrections), B3LYP/6-311+G(d) (in curly brackets, with ZPE corrections), and single-point CCSD(T)/6-311+G(d)//PBE0/6-311+G(d) levels (in square brackets), respectively. These isomeric structures are higher in energy with respect to the low-lying structures shown in Figure 2 in the main text.

Figure S1. Selected optimized sandwich- and helix-type isomeric structures of $Be_6B_7^-$ cluster at the PBE0/6-311+G(d) level along with their relative energies (in kcal mol^{-1}) above the GM structure, including zero-point energy (ZPE) corrections. Also presented are energetics data at the PBE0-D3/6-311+G(d) (in *italics*, with ZPE corrections), B3LYP/6-311+G(d) (in curly brackets, with ZPE corrections), and single-point CCSD(T)/6-311+G(d)//PBE0/6-311+G(d) levels (in square brackets), respectively. These isomeric structures are higher in energy with respect to the low-lying structures shown in Figure 2 in the main text.
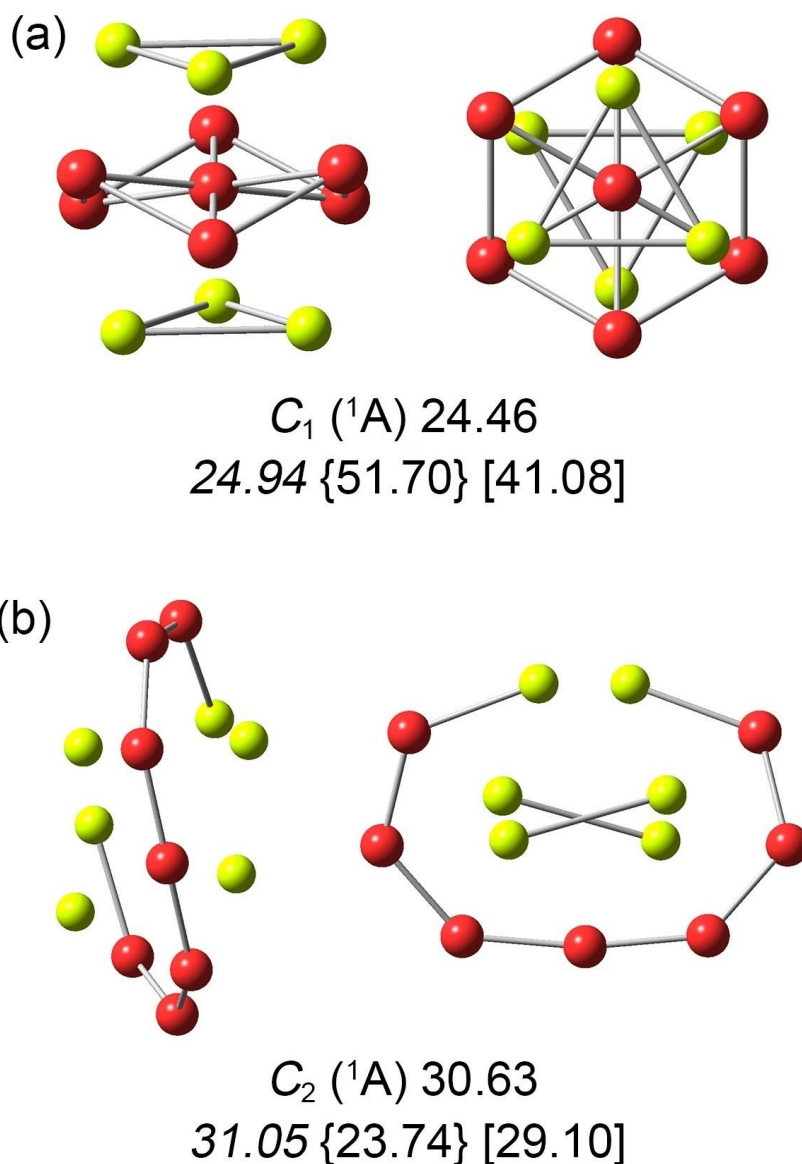
(a)

C_1 (^{1}A) 24.46
24.94 {51.70} [41.08]

(b)

C_2 (^{1}A) 30.63
31.05 {23.74} [29.10]

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(a) GM $Be_6B_7^-$ C_{2v} ($^1A_1$)

B	0.00000000	2.35737400	0.10635000
B	0.00000000	-1.55971000	1.44868100
B	0.00000000	1.55571000	-1.27108600
B	0.00000000	-2.35737400	0.10635000
B	0.00000000	0.00000000	1.72074100
B	0.00000000	-1.55571000	-1.27108600
B	0.00000000	1.55971000	1.44868100
Be	-0.98037100	0.00000000	-1.66425700
Be	-1.24860500	-1.03347100	0.11693100
Be	1.24860500	-1.03347100	0.11693100
Be	0.98037100	0.00000000	-1.66425700
Be	1.24860500	1.03347100	0.11693100
Be	-1.24860500	1.03347100	0.11693100

(b) Sandwich-type C_1 (^1A) structure

B	-0.00030200	-0.00001700	-0.00362100
B	-1.65887500	0.03030800	0.33698900
B	0.85949300	1.42095000	0.32729500
B	0.80488100	-1.45466000	0.31792600
B	-0.85982400	-1.42192800	-0.32639000
B	1.65947900	-0.03025400	-0.33547900

B	-0.80515900	1.45560000	-0.31701800
Be	-0.56123700	1.02657500	1.51164100
Be	-0.59955700	-1.01435900	1.50520900
Be	1.18641200	-0.02728200	1.49860400
Be	-1.18760400	0.02728300	-1.49810600
Be	0.56203400	-1.02697300	-1.51168800
Be	0.60033400	1.01475800	-1.50528800

(c) Helix-type C_2 (^{1}A) structure

Be	1.32849600	0.04551600	-0.32083600
Be	-1.32849600	-0.04551600	-0.32083600
Be	0.00000000	1.61001500	0.24741300
Be	0.00000000	-1.61001500	0.24741300
B	0.00000000	0.00000000	1.59528600
Be	0.06256500	1.05455300	-1.73444100
Be	-0.06256500	-1.05455300	-1.73444100
B	1.28724800	-0.87560100	1.45995800
B	-1.28724800	0.87560100	1.45995800
B	-1.92320100	1.71315600	0.30968100
B	1.92320100	-1.71315600	0.30968100
B	1.37457800	-1.87048800	-1.12099100
B	-1.37457800	1.87048800	-1.12099100