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

SUPPLEMENTARY INFORMSTION

Isovalent electronic systems B_{13}^+ and BeB_{12}: Structure interchange of GM and TS

Ceng Zhang,[a] Hai-ru Li,*[a] Rui-Hua Zhou,[a] Yan Zhang,[a] Xiong-Bo Duan*[b]

[a] School of Materials Science and Engineering, North University of China, Taiyuan, 030051, China.

E-mail: lihairu@nuc.edu.cn

[b] School of Energy Science and Engineering, Central South University, Changsha 410083, China.

E-mail: xiongbo_duan@csu.edu.cn

SUPPLEMENTARY INFORMATION – PART

Figure S1. Optimized structures of the C_s global minimum (GM) and C_s transition state (TS) of BeB_{12} at PBE0/6-311+G(d) level. The bond distances are indicated in Å

Figure S2. NBO charge analysis of the global minimum(GM) and rotational transition state(TS) structures of C_s BeB_{12} clusters

Figure S3. Molecular dynamics simulation curves of GM structure at 1500 K and 2600 K

Table S1. Cartesian coordinates for the global-minimum (GM) structure and transition states (TS) at the PBE0/6-311+G (d) level.

GIF1: A GIF extracted from the BOMD simulation for C_s BeB_{12}.

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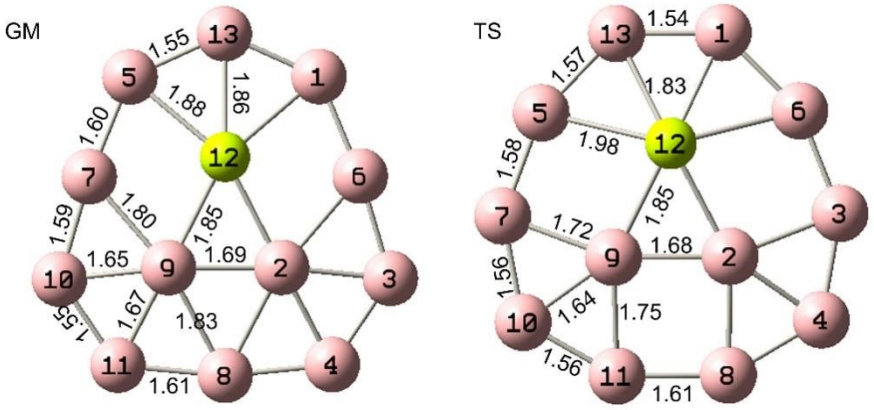

Figure S2. NBO charge analysis and WBIs of the global minimum(GM) and rotational transition state(TS) structures of BeB_{12} clusters

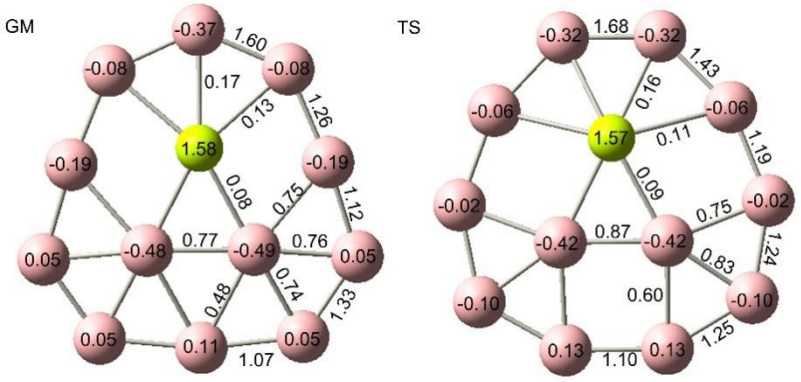

Figure S3. Molecular dynamics simulation curves of GM structure at 1500K and 2600K.

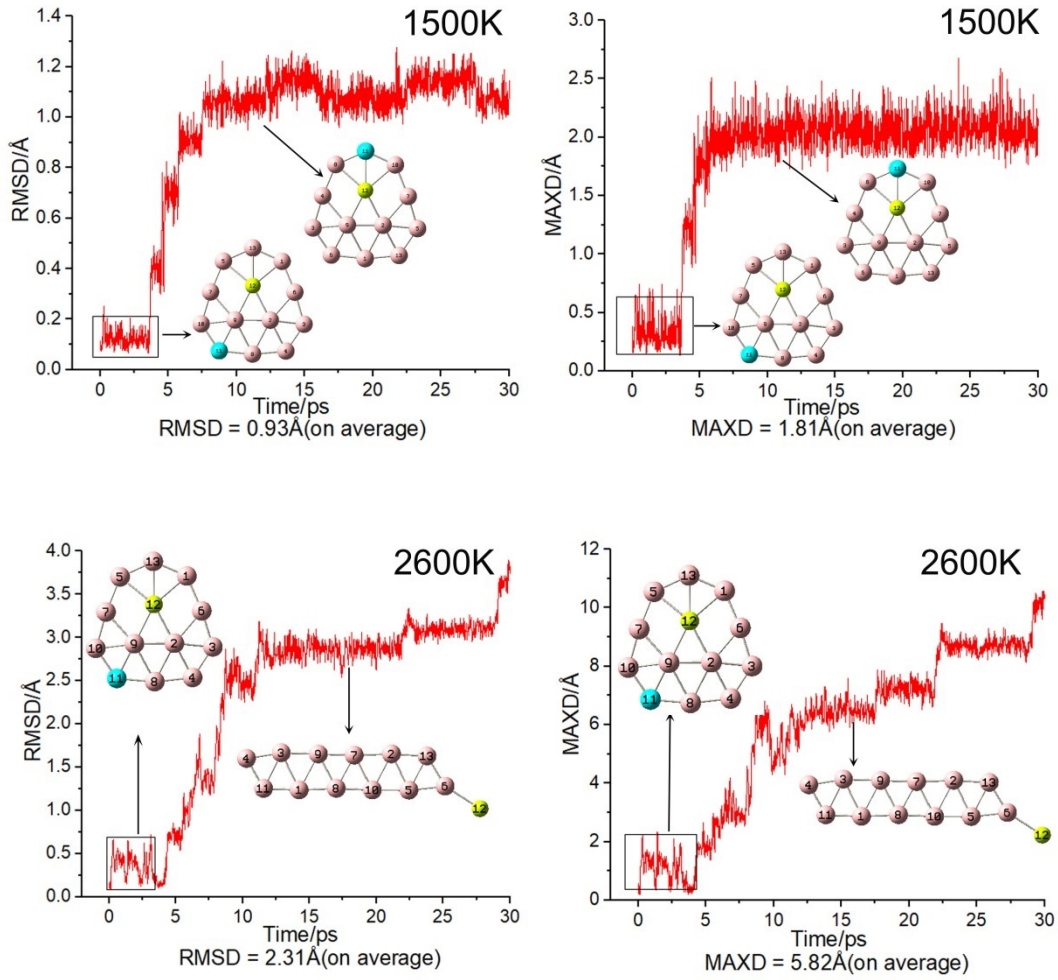

Table S1. Cartesian coordinates for the global-minimum (GM) structure and transition states (TS) at the PBE0/6-311+G(d) level.

(a) GM of C_s BeB_{12}

B	0.08100400	2.18231700	1.40790600
B	-0.19379300	-0.64612400	0.84368300
B	0.06175200	-0.82134000	2.46680500
B	0.09740100	-2.10146400	1.59843800
B	0.08100400	2.18231700	-1.40790600
B	-0.00835500	0.70453300	2.01955400
B	-0.00835500	0.70453300	-2.01955400
B	0.05626600	-2.25576600	0.00000000
B	-0.19379300	-0.64612400	-0.84368300
B	0.06175200	-0.82134000	-2.46680500
B	0.09740100	-2.10146400	-1.59843800
Be	-0.28758000	1.00046700	0.00000000
B	0.09778000	2.81955000	0.00000000

(b) TS of C_s BeB_{12}

B	2.59633800	-0.77021000	-0.12923400
B	-0.60653700	-0.84093900	0.25234900
B	-0.01134200	-2.42999900	-0.04050700
B	-1.54191200	-2.14826400	-0.08962100
B	1.46980800	1.86225300	-0.05772900
B	1.46706900	-1.86386200	-0.05714500
B	-0.00813400	2.42965600	-0.04031900
B	-2.32215700	-0.80111900	-0.11005500
B	-0.60544000	0.84156000	0.25222900
B	-1.53920300	2.15020300	-0.08929200

B	-2.32106400	0.80408200	-0.10979900
Be	1.03140400	-0.00040000	0.43581100
B	2.59745200	0.76696000	-0.12952600

GIF1: A GIF extracted from the BOMD simulation for BeB_{12}

BeB12.gif