

Electronic Supplementary Information 1

## **CBe<sub>4</sub>H<sub>6</sub>: A molecular rotor with a built-in on-off switch**

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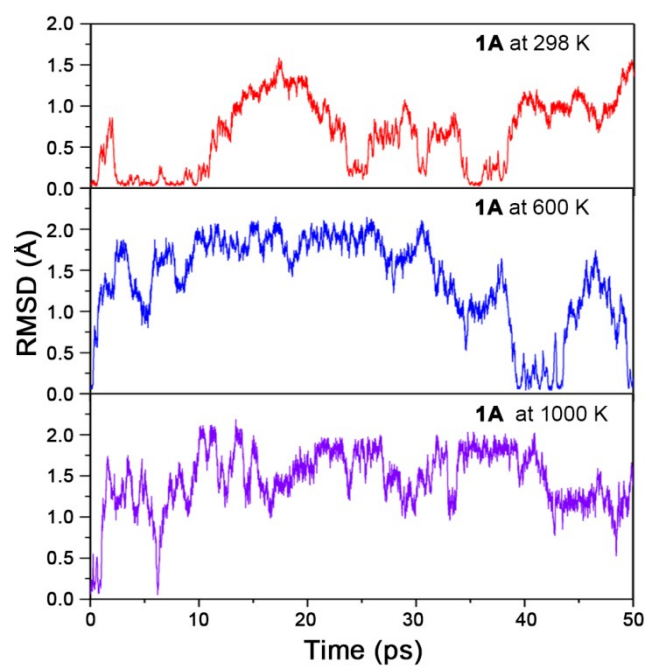
E-mail: [wbyb@sxu.edu.cn](mailto:wbyb@sxu.edu.cn) (Y.B.W.)

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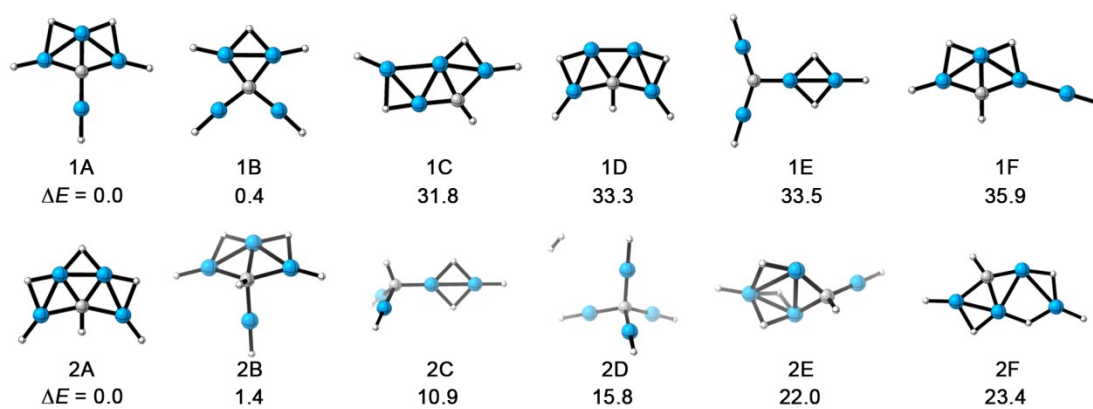
**Fig. S1** Plots of root-mean-square deviation (RMSD, in Å and relative to the PBE/DZVP-optimized structures) for 50 pico-second (ps) BOMD simulations of CBe<sub>4</sub>H<sub>5</sub><sup>-</sup> system (starting from **1A**) at the PBE/DZVP level.

**Fig. S2** Structures and relative energies ( $\Delta E$ , in kcal/mol at the CCSD(T)//B2PLYP level) of CBe<sub>4</sub>H<sub>5</sub><sup>-</sup> and CBe<sub>4</sub>H<sub>6</sub> and their lowest-lying isomers.

Cartesian coordinates of B2PLYP-D3(BJ)/aug-cc-pVTZ-optimized structures shown in Fig. 1 and Fig. S2.



**Fig. S1** Plots of root-mean-square deviation (RMSD, in Å and relative to the PBE/DZVP-optimized structures) for 50 pico-second (ps) BOMD simulations of  $\text{CBe}_4\text{H}_5^-$  system (starting from **1A**) at the PBE/DZVP level.



**Fig. S2** Structures and relative energies ( $\Delta E$ , in kcal/mol at the CCSD(T)//B2PLYP level) of  $\text{CBe}_4\text{H}_5^-$  and  $\text{CBe}_4\text{H}_6$  and their lowest-lying isomers.

Cartesian coordinates of B2PLYP-D3(BJ)/aug-cc-pVTZ-optimized structures shown in Fig. 1 and Fig. S2.

**0**

C	0.00000000	0.00000000	0.00000000
Be	0.00000000	1.14790900	1.14567300
Be	0.00000000	-1.14790900	1.14567300
Be	0.00000000	-1.14790900	-1.14567300
Be	0.00000000	1.14790900	-1.14567300
H	0.00000000	2.06373700	2.13244100
H	0.00000000	2.06373700	-2.13244100
H	0.00000000	-2.06373700	-2.13244100
H	0.00000000	-2.06373700	2.13244100

**1A**

C	0.00000000	0.00000000	0.21574100
Be	0.00000000	0.00000000	1.80653800
Be	0.00000000	1.60227200	-0.27294000
Be	0.00000000	0.00000000	-1.42665600
Be	0.00000000	-1.60227200	-0.27294000
H	0.00000000	2.93273100	0.03392400
H	0.00000000	1.31612800	-1.92778200
H	0.00000000	-1.31612800	-1.92778200
H	0.00000000	-2.93273100	0.03392400
H	0.00000000	0.00000000	3.15726600

**1B**

C	0.00000000	0.00000000	0.18470600
Be	0.00000000	1.26503900	1.15609300
Be	0.00000000	1.00182800	-1.16768800
Be	0.00000000	-1.00182800	-1.16768800
Be	0.00000000	-1.26503900	1.15609300
H	0.00000000	2.34212800	-1.44600300
H	0.00000000	0.00000000	-2.26669400
H	0.00000000	-2.34212800	-1.44600300
H	0.00000000	-2.25574300	2.07160800
H	0.00000000	2.25574300	2.07160800

**TS1**

C	0.00000000	0.19980600	0.00000000
Be	1.59974800	0.45910700	0.00000000
Be	0.51783700	-1.38262700	0.00000000
Be	-1.37218800	-0.77462800	0.00000000
Be	-0.72782100	1.61366400	0.00000000

H	1.83392800	-1.78469100	0.00000000
H	-0.69532900	-2.16914500	0.00000000
H	-2.73941500	-0.75411900	0.00000000
H	-1.30424700	2.83380100	0.00000000
H	2.83475600	1.01324900	0.00000000

### 1C

C	-0.76463300	0.73729000	0.00004200
Be	2.22275300	-0.52887300	0.00013800
Be	-0.00154200	-0.76770800	-0.00020000
Be	-1.93121800	-0.53435000	-0.00000900
Be	0.85944900	0.92192000	0.00005800
H	2.25565100	1.14235100	-0.00016700
H	-1.02893300	-1.76827300	-0.00020800
H	-3.28762900	-0.70850100	-0.00001700
H	3.48133400	-1.05066000	0.00012300
H	-1.43039600	1.59739100	0.00006700

### 1D

C	0.00000000	-0.25250500	-0.00020900
Be	-0.94341200	1.19346400	0.00003300
Be	0.94340800	1.19346200	-0.00004800
Be	1.70296700	-0.60491100	0.00015400
Be	-1.70296500	-0.60491400	0.00012100
H	2.31063900	0.78557200	0.00021500
H	-2.50618000	-1.70141900	0.00014600
H	2.50618100	-1.70141600	0.00022900
H	0.00000300	-1.36167900	-0.00063000
H	-2.31064100	0.78556700	0.00025300

### 1E

C	-0.98143300	-0.00077900	-0.00026900
Be	-1.39095700	1.53034700	0.00013700
Be	2.62766800	0.00297400	0.00006500
Be	-1.38321900	-1.53400500	0.00011400
Be	0.62445600	0.00112100	-0.00014300
H	1.70993300	1.08519600	-0.00030200
H	-1.71799400	2.84728900	0.00046000
H	-1.70335800	-2.85263400	0.00032400
H	1.71189700	-1.08092700	0.00018300
H	3.97632700	0.00399200	0.00025700

### 1F

C	0.52848400	-0.58282700	0.00017800
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Be	2.20962200	-0.25783400	-0.00000600
Be	0.76237900	1.00801700	0.00018500
Be	-3.05249500	-0.13141700	-0.00010900
Be	-0.98988400	0.20519700	-0.00026500
H	-4.39911900	-0.37376000	0.00028700
H	3.46149400	-0.81001900	-0.00074200
H	2.14386800	1.33357500	0.00010500
H	-0.47510700	1.70604100	-0.00014600
H	0.37947400	-1.65472400	0.00021600

## 2A

C	0.00000000	0.00000000	0.30648000
H	0.00000000	2.54191500	1.74756300
H	0.00000000	-2.54191500	1.74756300
Be	0.00000000	1.74585300	0.68164600
Be	0.00000000	0.94265700	-1.05815000
Be	0.00000000	-0.94265700	-1.05815000
Be	0.00000000	-1.74585300	0.68164600
H	0.00000000	2.29903100	-0.78434000
H	0.00000000	0.00000000	-2.15484600
H	0.00000000	-2.29903100	-0.78434000
H	0.00000000	0.00000000	1.40155200

## 2B

C	0.21774000	0.35460200	0.00000000
H	0.15639900	0.12995500	2.93118900
H	-2.20185500	2.08667700	0.00000000
Be	0.21774000	-0.24744300	1.65450000
Be	0.44717200	-1.32562000	0.00000000
Be	0.21774000	-0.24744300	-1.65450000
Be	-1.14143900	1.29664900	0.00000000
H	0.35508700	-1.79634900	1.31362800
H	0.35508700	-1.79634900	-1.31362800
H	0.15639900	0.12995500	-2.93118900
H	0.90759300	1.21392500	0.00000000

## TS2

C	0.01634500	-0.22655600	0.33980400
H	2.43438600	1.08551600	-0.14440100
H	2.16888400	-2.07260000	-0.58128900
Be	1.11425100	1.08206500	0.09000500
Be	-0.83559600	1.15763400	-0.08344000
Be	-1.63446400	-0.64136300	-0.13973200
Be	1.31037000	-1.12235200	-0.24708700

H	0.13686600	2.14037500	-0.40669200
H	-2.14618800	0.84988000	-0.43654000
H	-2.50020100	-1.65309700	-0.16457100
H	-0.01006000	-0.89467300	1.21568600

**2<sup>nd</sup>SP**

C	-0.33488000	-0.18635000	0.00000000
H	0.37947900	1.15272400	2.31384500
H	0.34518300	-1.98492900	2.27323000
Be	0.09866500	1.18095400	0.99944900
Be	0.09866500	1.18095400	-0.99944900
Be	0.09866500	-1.06311900	-1.35526100
Be	0.09866500	-1.06311900	1.35526100
H	0.40888900	2.21239900	0.00000000
H	0.37947900	1.15272400	-2.31384500
H	0.34518300	-1.98492900	-2.27323000
H	-1.42757900	-0.37257800	0.00000000

**2C**

C	-0.82374400	-0.00006500	0.43756100
Be	-1.49411300	-1.32767900	-0.25224700
Be	-1.49394000	1.32789200	-0.25173900
Be	2.76612300	-0.00013000	-0.17461900
Be	0.80611000	-0.00004900	0.16949300
H	1.60911900	0.00109500	-1.06458700
H	4.07070000	-0.00003100	-0.40737600
H	-2.01050500	-2.39899000	-0.84331300
H	-2.00937600	2.39963100	-0.84286500
H	1.98109600	-0.00096800	1.05372100
H	-1.03529000	-0.00048300	1.51550400

**2D**

C	-0.27971700	-0.00031600	0.00009600
Be	0.66371500	-1.32882900	-0.01267600
Be	0.65962000	1.33100400	0.02279400
Be	-1.21438100	0.01685100	-1.33388100
Be	-1.22911900	-0.01920400	1.32358700
H	1.41272900	2.42175000	0.04125700
H	-1.97462700	0.03094000	-2.41957400
H	1.42026000	-2.41729300	-0.02325100
H	3.65052900	-0.36974600	-0.00565400
H	-2.00137600	-0.03455200	2.40075300
H	3.65145200	0.37150900	0.00660700

**2E**

C	0.94459700	0.28526300	0.43037500
Be	-0.41737600	-0.71629200	0.60135900
Be	2.16242100	-0.37957400	-0.44098900
Be	-0.19626800	1.10321700	-0.39665600
Be	-2.15631200	-0.24670200	-0.23306000
H	3.11862800	-0.94313600	-1.17292600
H	-1.67338400	-0.31843300	1.19532200
H	-1.51413400	1.18554800	-0.77506700
H	-3.42669300	-0.34086400	-0.63043800
H	-1.03706300	-1.14960100	-0.64461400
H	1.29520100	0.81230600	1.32285700

**2F**

C	-0.76017100	0.70058600	0.00305900
Be	2.37086400	-0.42285900	0.00786100
Be	-2.05743700	-0.48513600	0.00485500
Be	-0.16127500	-0.81112000	-0.01101000
Be	0.75888400	1.12608300	-0.01344200
H	1.20088300	-1.22264200	-0.03592700
H	-3.39280800	-0.53497400	0.01607900
H	-1.18620300	-1.76731100	-0.00922800
H	-1.45851000	1.53145800	0.02590200
H	2.13647200	1.02953200	-0.01531700
H	3.61705100	-0.86745300	0.04708500