SUPPLEMENTARY INFORMATION

The Unique Sandwich $K_6Be_2B_6H_6$ Cluster with a Real Borozene B_6H_6 Core†

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Supplementary Information – Part I

Table S1. Cartesian coordinates for selected structures of $K_6Be_2B_6H_6$ cluster at the PBE0/6-311+G(d,p) level: D_{3d} ($^1A_{1g}$) global-minimum (GM), D_{3h} ($^1A_1'$) low-lying isomer (LM), and two transition state (TS) structures of D_{3d} ($^1A_{1g}$) TS_1 and D_{3h} ($^1A_1'$) TS_2.

Figure S1. Alternative optimized isomers of $K_6Be_2B_6H_6$ cluster. Relative energies are shown in square brackets at the PBE0/6-311+G(d,p) level with corrections for zero-point energies (ZPEs). Also shown are the relative energies for top five isomers at the single-point CCSD(T)/6-311+G(d,p)//PBE0/6-311+G(d,p) level. All energies are in eV.

Figure S2. Wiberg bond indices (WBIs) (a/c) and natural atomic charges (b/d, in |e|) for GM (D_{3d}, $^1A_{1g}$) and LM (D_{3h}, $^1A_1'$) isomers of $K_6Be_2B_6H_6$ cluster from the natural bond orbital (NBO) analyses at the PBE0/6-311+G(d,p) level.

Figure S3. Occupied canonical molecular orbitals (CMOs) of D_{3h} ($^1A_1'$) LM for $K_6Be_2B_6H_6$ cluster. (a) Six σ CMOs for six B–B σ bonds. (b) Six σ CMOs for six B–H σ bonds. (c) Three delocalized π CMOs on B_6H_6 ring. (d) Two σ CMOs over two tetrahedral K_3Be ligands.

Figure S4. Adaptive natural density partitioning (AdNDP) bonding pattern of D_{3h} ($^1A_1'$) LM for $K_6Be_2B_6H_6$ cluster. Occupation numbers (ONs) are indicated.

Figure S5. Displacement vectors for the soft vibrational modes of (a) D_{3d} ($^1A_{1g}$) GM and (b) D_{3h} ($^1A_1'$) LM structures for $K_6Be_2B_6H_6$ cluster.

Supplementary Information – Part II

A short movie extracted from the BOMD simulation for $K_6Be_2B_6H_6$ cluster. The simulation was performed at the temperature of 300 K for 10 ps, starting from the equilibrium GM structure with random atom velocities. The movie roughly covers a time span of 4.2 ps.

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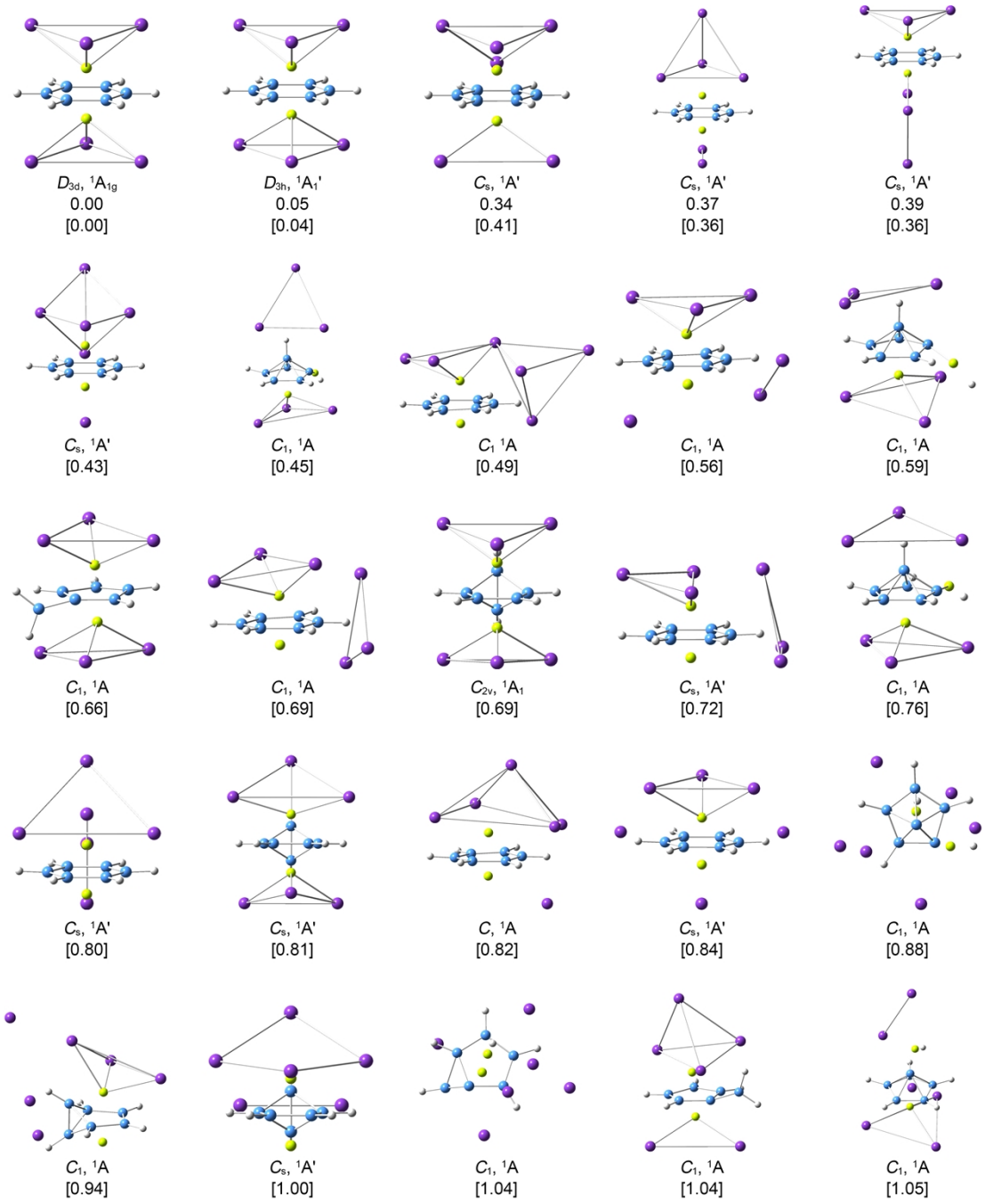

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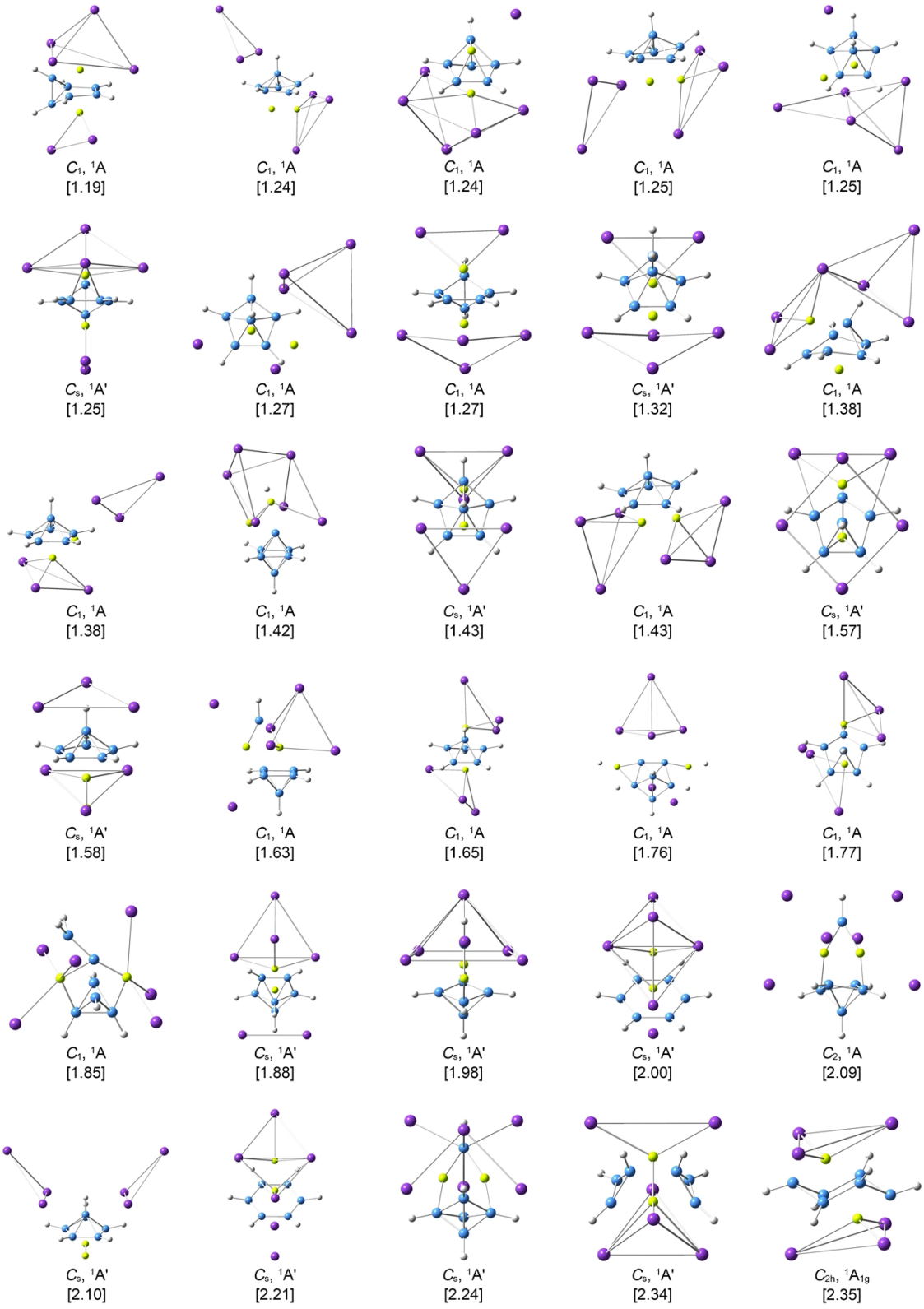
C_1, ^{1}A
[1.19]
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C_1, ^{1}A
[1.25]
C_s, ^{1}A'
[1.25]
C_1, ^{1}A
[1.27]
C_1, ^{1}A
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C_1, ^{1}A
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[2.09]
C_s, ^{1}A'
[2.10]
C_s, ^{1}A'
[2.21]
C_s, ^{1}A'
[2.24]
C_s, ^{1}A'
[2.34]
C_{2h}, ^{1}A$_{1g}$
[2.35]

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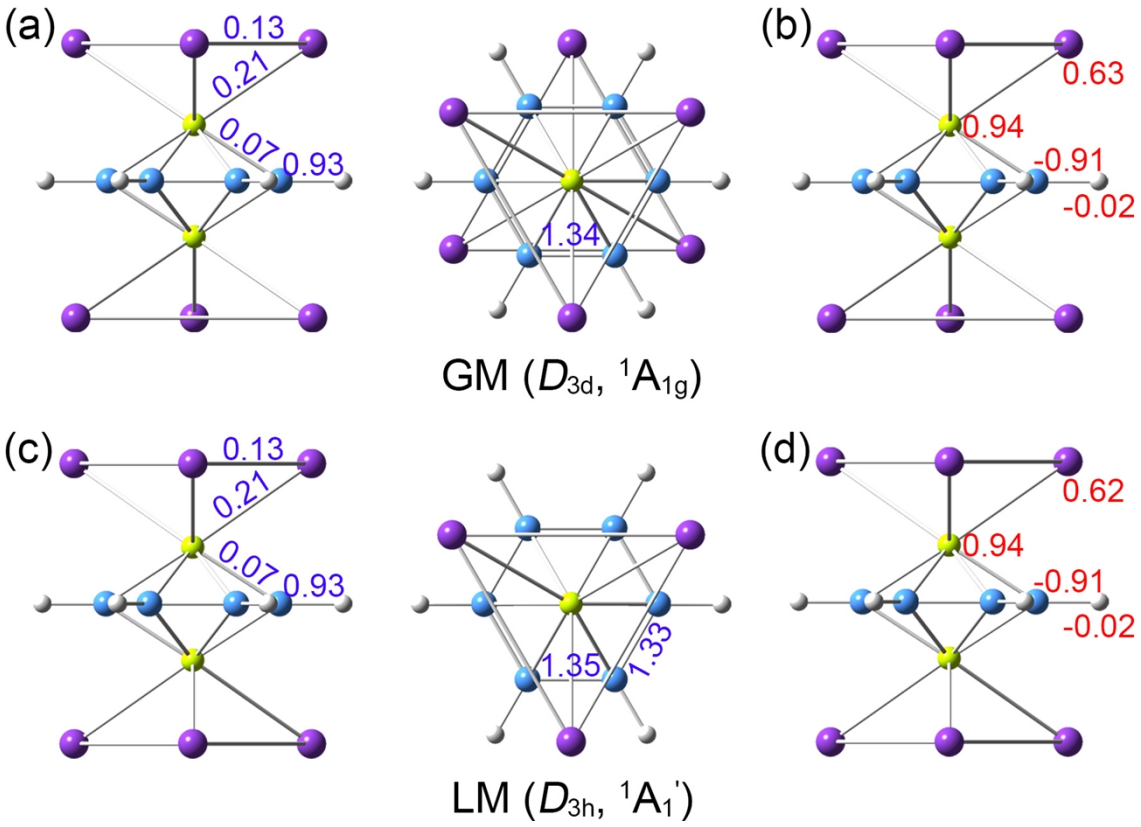

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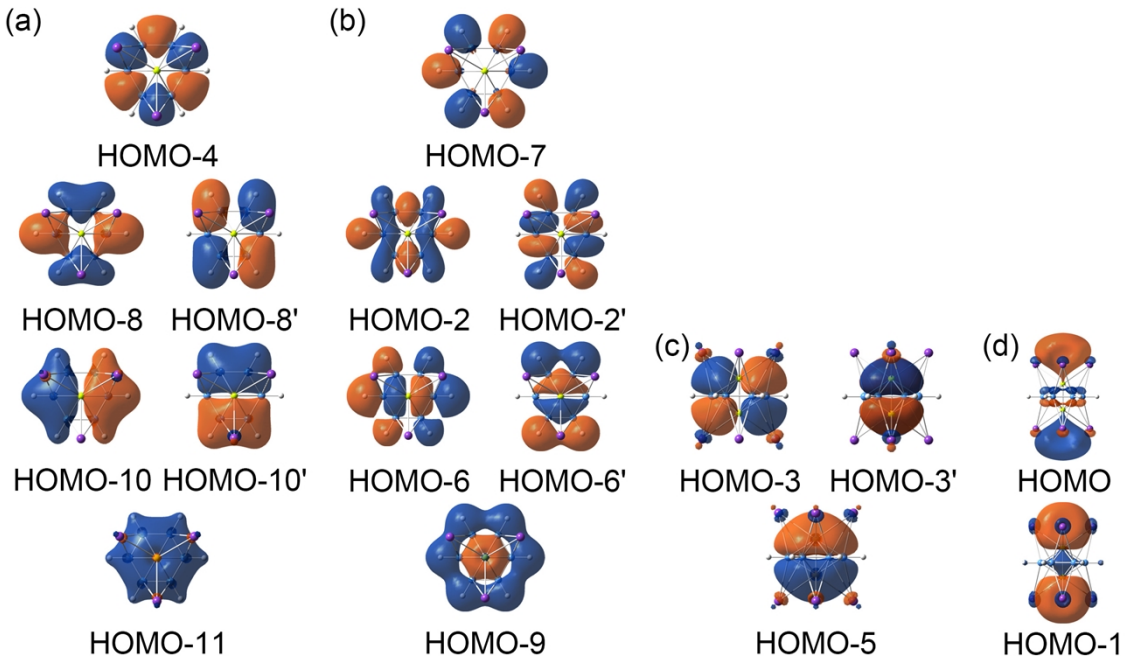

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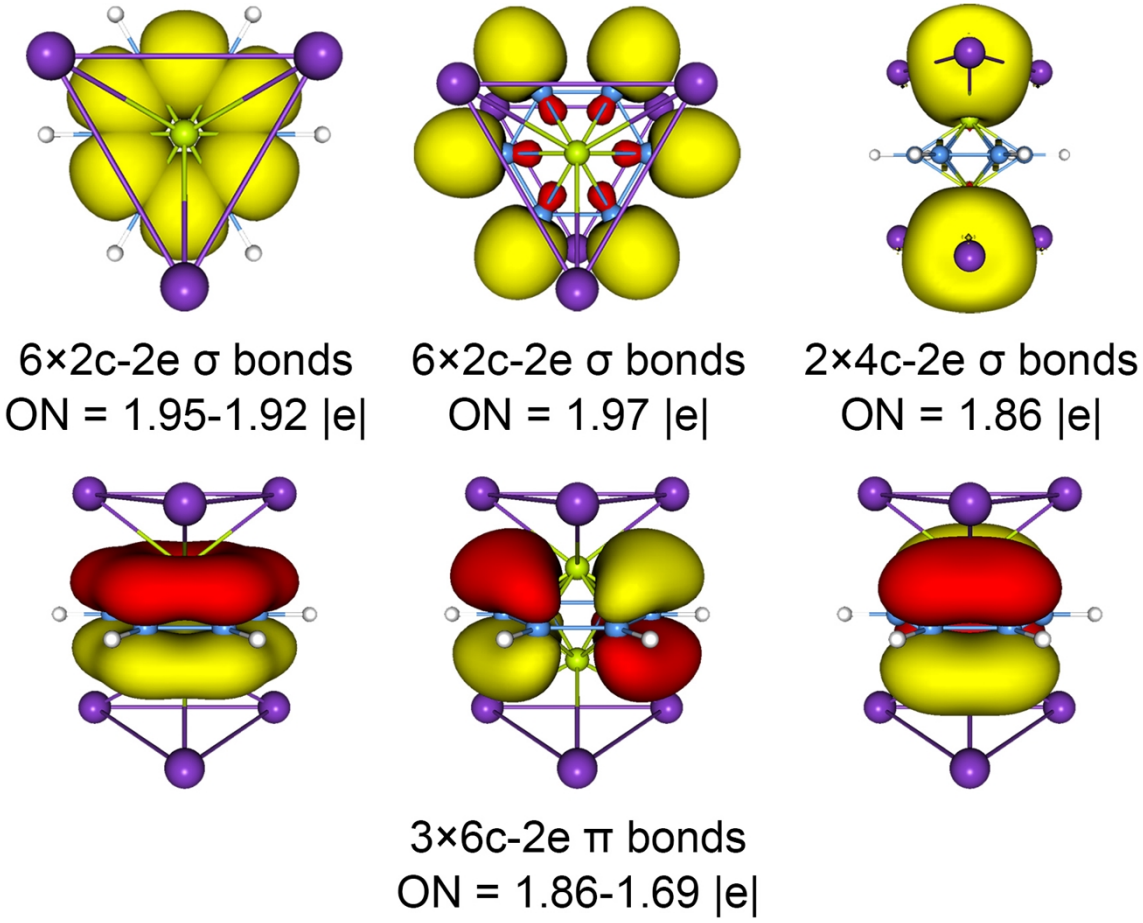

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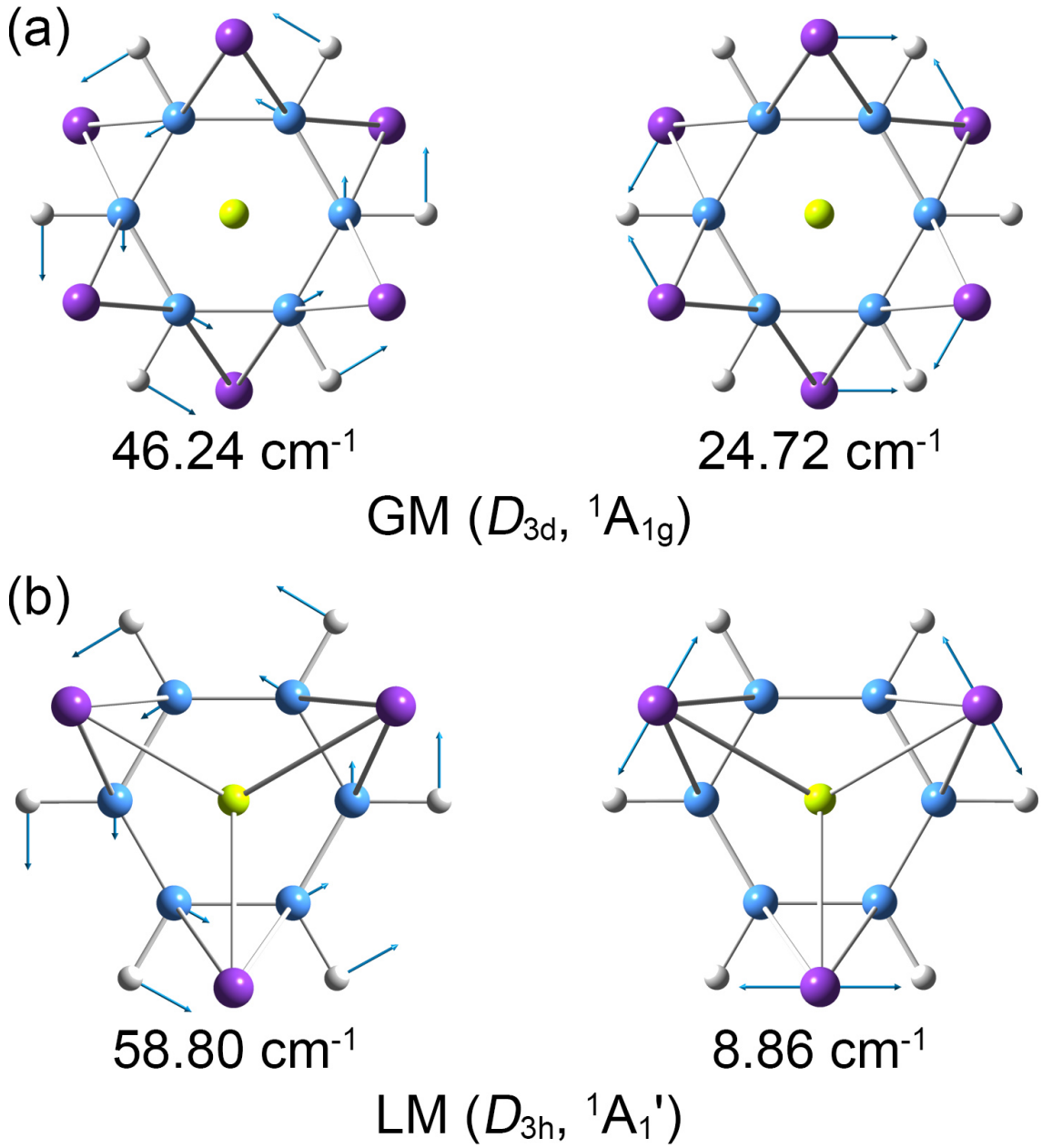

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$K_6Be_2B_6H_6$ GM (D_{3d}, $^1A_{1g}$)

B	0.83544400	1.44703100	0.00000000
B	1.67088800	0.00000000	0.00000000
B	0.83544400	-1.44703100	0.00000000
B	-0.83544400	1.44703100	0.00000000
B	-1.67088800	0.00000000	0.00000000
B	-0.83544400	-1.44703100	0.00000000
H	-1.44802200	-2.50804700	0.00000000
H	-2.89604300	0.00000000	0.00000000
H	-1.44802200	2.50804700	0.00000000
H	1.44802200	2.50804700	0.00000000
H	2.89604300	0.00000000	0.00000000
H	1.44802200	-2.50804700	0.00000000
Be	0.00000000	0.00000000	1.08940500
Be	0.00000000	0.00000000	-1.08940500
K	-2.30689500	-1.33188700	2.66900000
K	-2.30689500	1.33188700	-2.66900000
K	0.00000000	2.66377300	2.66900000
K	2.30689500	-1.33188700	2.66900000
K	2.30689500	1.33188700	-2.66900000
K	0.00000000	-2.66377300	-2.66900000

$K_6Be_2B_6H_6$ LM (D_{3h}, $^1A_1'$)

B	-0.83355300	1.44936300	0.00000000

B	0.83355300	1.44936300	0.00000000
B	1.67196100	-0.00280400	0.00000000
B	0.83840900	-1.44655900	0.00000000
B	-0.83840900	-1.44655900	0.00000000
B	-1.67196100	-0.00280400	0.00000000
H	1.45616200	-2.50482100	0.00000000
H	2.89731900	-0.00866300	0.00000000
H	1.44115800	2.51348300	0.00000000
H	-1.44115800	2.51348300	0.00000000
H	-2.89731900	-0.00866300	0.00000000
H	-1.45616200	-2.50482100	0.00000000
Be	0.00000000	0.00000000	1.08745000
Be	0.00000000	0.00000000	-1.08745000
K	2.28679900	1.32028400	-2.69435400
K	-2.28679900	1.32028400	-2.69435400
K	0.00000000	-2.64056800	-2.69435400
K	-2.28679900	1.32028400	2.69435400
K	2.28679900	1.32028400	2.69435400
K	0.00000000	-2.64056800	2.69435400

$K_6Be_2B_6H_6$ TS_1 (D_{3d}, $^1A_{1g}$)

B	0.00000000	-1.67434600	0.02326300
B	1.45002600	-0.83717300	-0.02326300
B	1.45002600	0.83717300	0.02326300
B	-1.45002600	-0.83717300	-0.02326300
B	-1.45002600	0.83717300	0.02326300
B	0.00000000	1.67434600	-0.02326300
H	0.00000000	2.89742500	0.00526300
H	-2.50924400	1.44871300	-0.00526300

H	-2.50924400	-1.44871300	0.00526300
H	0.00000000	-2.89742500	-0.00526300
H	2.50924400	-1.44871300	0.00526300
H	2.50924400	1.44871300	-0.00526300
Be	0.00000000	0.00000000	1.08139700
Be	0.00000000	0.00000000	-1.08139700
K	2.25832700	1.30384600	-2.75013600
K	-2.25832700	1.30384600	-2.75013600
K	0.00000000	2.60769200	2.75013600
K	2.25832700	-1.30384600	2.75013600
K	0.00000000	-2.60769200	-2.75013600
K	-2.25832700	-1.30384600	2.75013600

$K_6Be_2B_6H_6$ TS_2 (D_{3h}, $^1A_1'$)

B	-1.46220300	0.84420300	0.00000000
B	0.00000000	1.66241600	0.00000000
B	1.46220300	0.84420300	0.00000000
B	-1.43969400	-0.83120800	0.00000000
B	0.00000000	-1.68840700	0.00000000
B	1.43969400	-0.83120800	0.00000000
H	2.50681000	-1.44730800	0.00000000
H	0.00000000	-2.90277000	0.00000000
H	-2.50681000	-1.44730800	0.00000000
H	-2.51387300	1.45138500	0.00000000
H	0.00000000	2.89461500	0.00000000
H	2.51387300	1.45138500	0.00000000
Be	0.00000000	0.00000000	1.07790100
Be	0.00000000	0.00000000	-1.07790100
K	2.24381600	-1.29546800	2.78732900
K	-2.24381600	-1.29546800	-2.78732900

K	-2.24381600	-1.29546800	2.78732900
K	0.00000000	2.59093500	2.78732900
K	0.00000000	2.59093500	-2.78732900
K	2.24381600	-1.29546800	-2.78732900