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

Supporting Information

Saturn-Like Charge-Transfer Complexes $Li_4\&B_{36}$, $Li_5\&B_{36}^{+}$, and $Li_6\&B_{36}^{2+}$: Exohedral Metalloborospherenes with A Perfect Cage-Like B_{36}^{4-} Core**

Wen-Juan Tian,[a] Qiang Chen,[a] Hai-Ru Li,[a] Miao Yan,[a] Yue-Wen Mu,[a] Hai-Gang Lu,*[a] Hua-Jin Zhai*[a] and Si-Dian Li *[a]

Complete citation of ref. 29.

Figure S1. Typical isomers of B_{36}^{4-} at the PBE0/6-311+G* level. The relative energies are indicated in eV.

Figures S2-S4. Low-lying isomers of Li_4B_{36}, $Li_5B_{36}^{+}$ and $Li_6B_{36}^{2+}$ at the PBE0/6-311+G* level. Their relative energies are indicated in eV. Also shown are the relative energies at the single-point CCSD(T)// PBE0/6-311+G* (in bracket).

Figure S5. Frontier molecular orbital of D_{2h} $Li_4\&B_{36}$ (**2**), C_{2v} $Li_5\&B_{36}^{+}$ (**3**), and T_h $Li_6\&B_{36}^{2+}$ (**4**) at the PBE0/6-311+G* level.

Figures S6-S8. Born-Oppenheimer molecular dynamics simulations of D_{2h} $Li_4\&B_{36}$ (**2**), C_{2v} $Li_5\&B_{36}^{+}$ (**3**), and T_h $Li_6\&B_{36}^{2+}$ (**4**) at (a) 200K, (b) 400K, (c) 600K and (d) 800K for 30 ps, respectively. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

Figure S9. Simulated (a) IR and (b) Raman spectra of D_{2h} $Li_4\&B_{36}$ (**2**), C_{2v} $Li_5\&B_{36}^{+}$ (**3**), and T_h $Li_6\&B_{36}^{2+}$ (**4**) compared with that of T_h B_{36}^{4-} (**1**) at the PBE0/6-311+G* level.

Table S1. The optimized coordinates of T_h B_{36}^{4-} (**1**), D_{2h} $Li_4\&B_{36}$ (**2**), C_{2v} $Li_5\&B_{36}^{+}$ (**3**), T_h $Li_6\&B_{36}^{2+}$ (**4**), D_{2h} $Li_2\&[Ca@B_{36}]$ (**5**), C_{2v} $Li_3\&[Ca@B_{36}]^{+}$ (**6**), and D_{2h} $Li_4\&[Ca@\ B_{36}]^{2+}$ (**7**) at the PBE0/6-311+G* level.

Complete citation of ref. 29

29 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09*, revision D.01, Gaussian, Inc., Wallingford, CT, 2009.

Figure S1. Typical isomers of B_{36}^{4-} at the PBE0/6-311+G* level. The relative energies are indicated in eV.

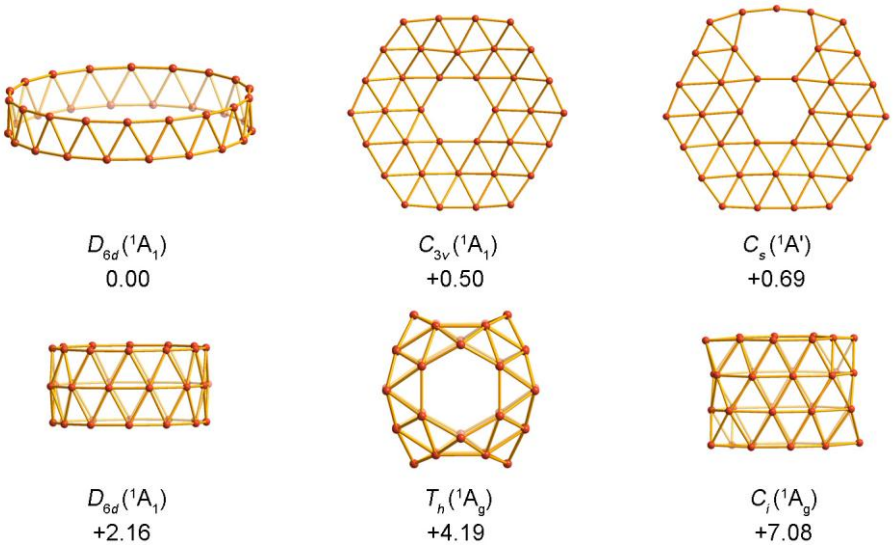
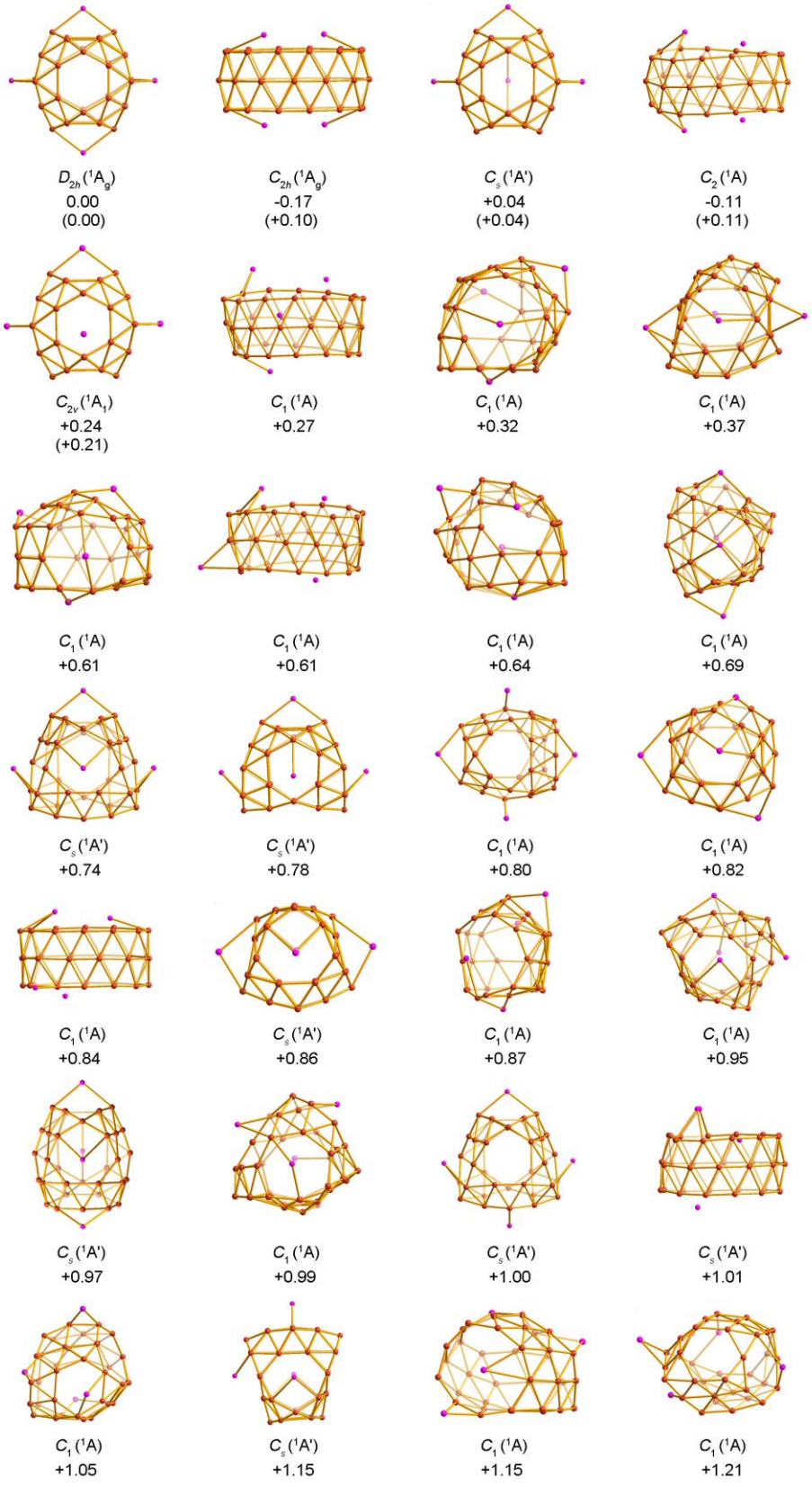


Figure S2. Low-lying isomers of Li_4B_{36} at the PBE0/6-311+G* level. Their relative energies are indicated in eV. Also shown are the relative energies at the single-point CCSD(T)// PBE0/6-311+G* (in bracket).



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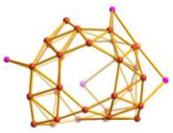

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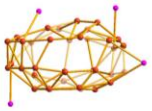

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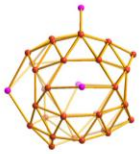

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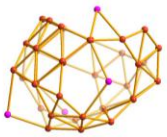

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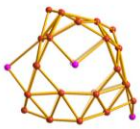

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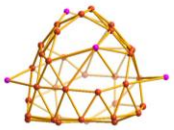

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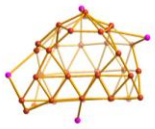

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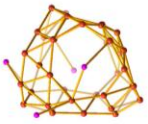

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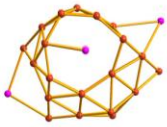

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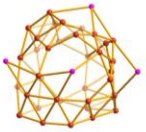

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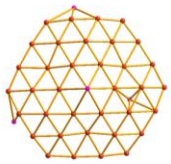

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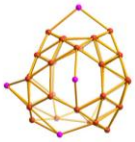

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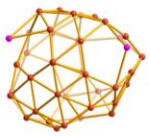

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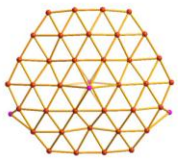

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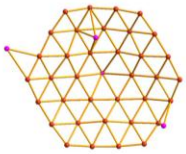

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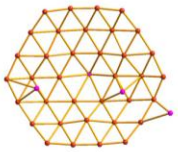

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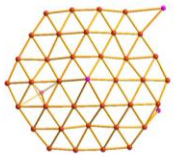

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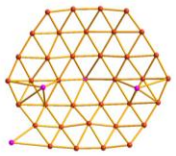

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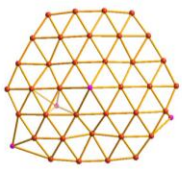

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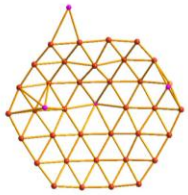

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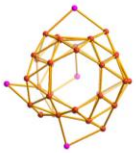

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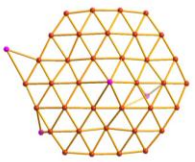

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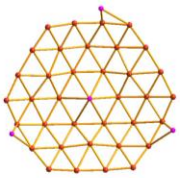

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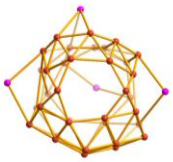

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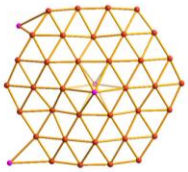

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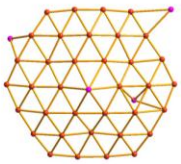

C_1 (^{1}A)
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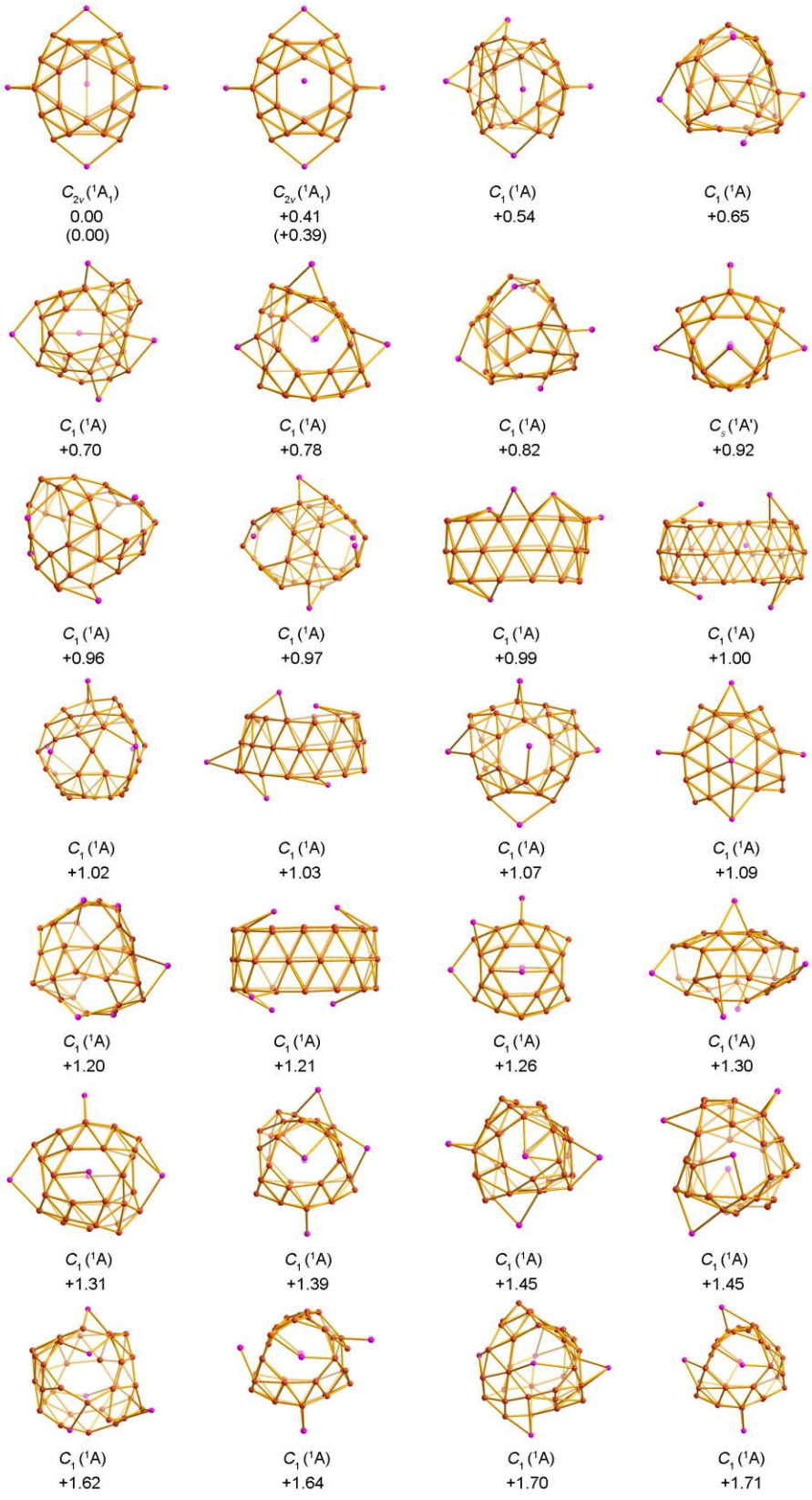
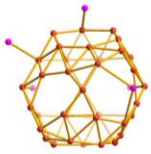
Figure S3. Low-lying isomers of $Li_5B_{36}^+$ at the PBE0/6-311+G* level. Their relative energies are indicated in eV. Also shown are the relative energies at the single-point CCSD(T)// PBE0/6-311+G* (in bracket).





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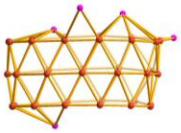

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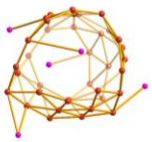

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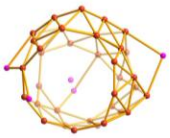

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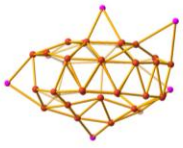

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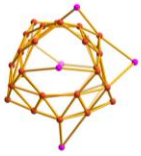

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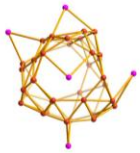

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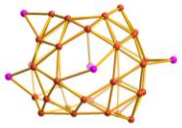

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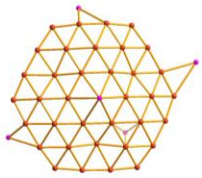

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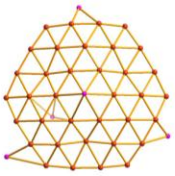

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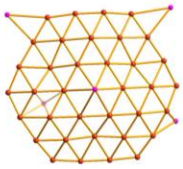

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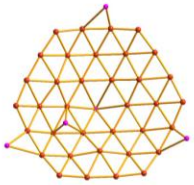

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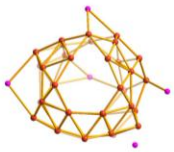

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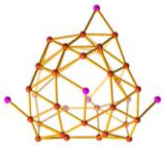

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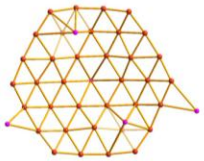

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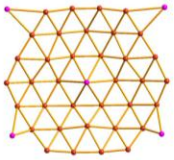

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+2.42

Figure S4. Low-lying isomers of $Li_6B_{36}^{2+}$ at the PBE0/6-311+G* level. Their relative energies are indicated in eV. Also shown are the relative energies at the single-point CCSD(T)// PBE0/6-311+G* (in bracket).

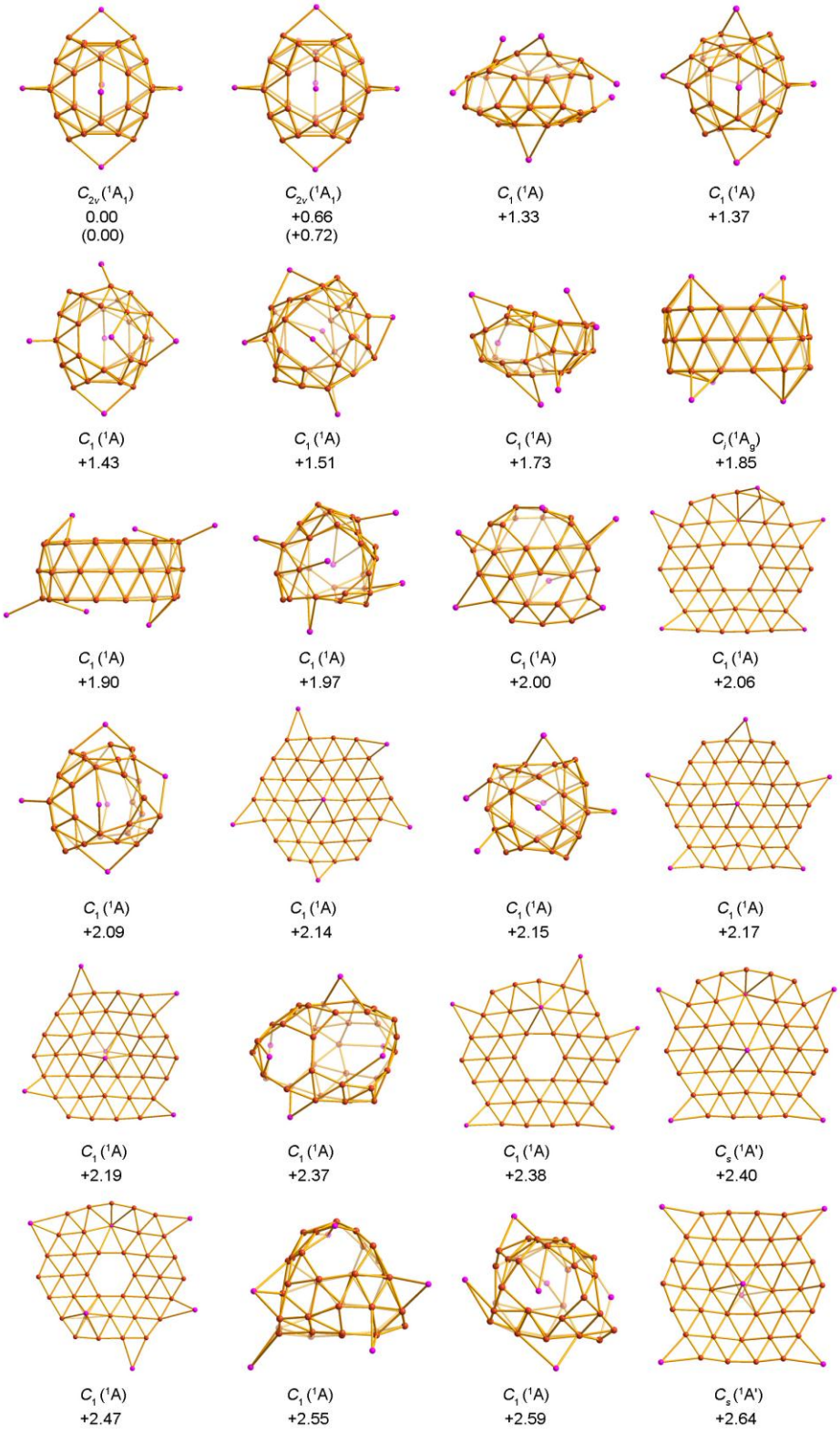

Figure S5. Frontier molecular orbital of D_{2h} $Li_4\&B_{36}$ (**2**), C_{2v} $Li_5\&B_{36}^{+}$ (**3**), and T_h $Li_6\&B_{36}^{2+}$ (**4**) at the PBE0/6-311+G* level.

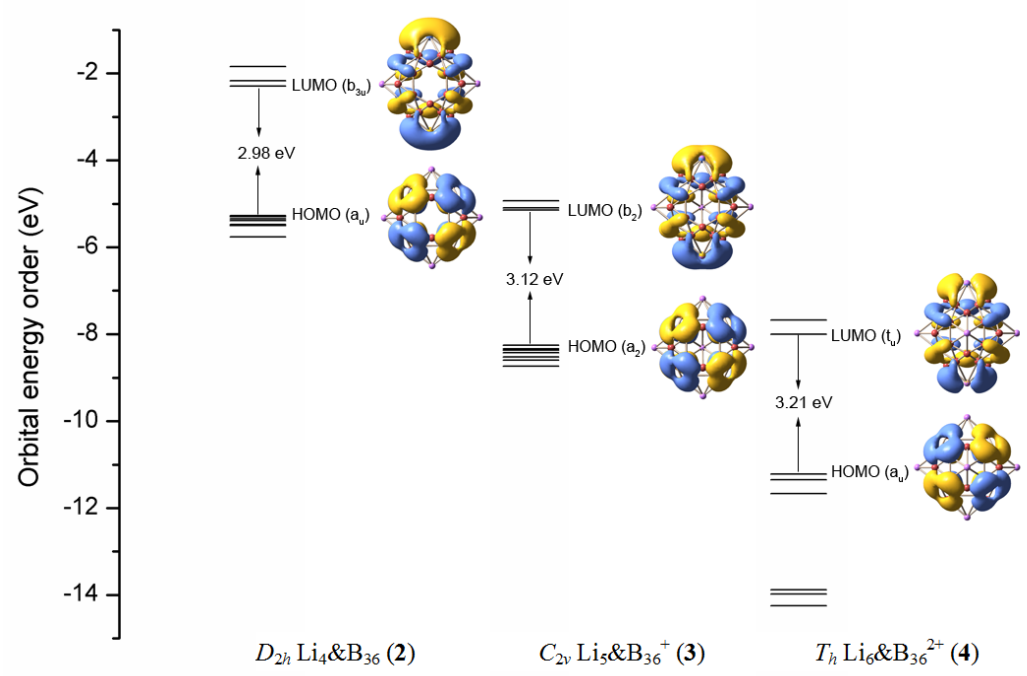

Figure S6. Born-Oppenheimer molecular dynamics simulations of D_{2h} $Li_4\&B_{36}$ (**2**) at (a) 200K, (b) 400K, (c) 600K and (d) 800K for 30 ps. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

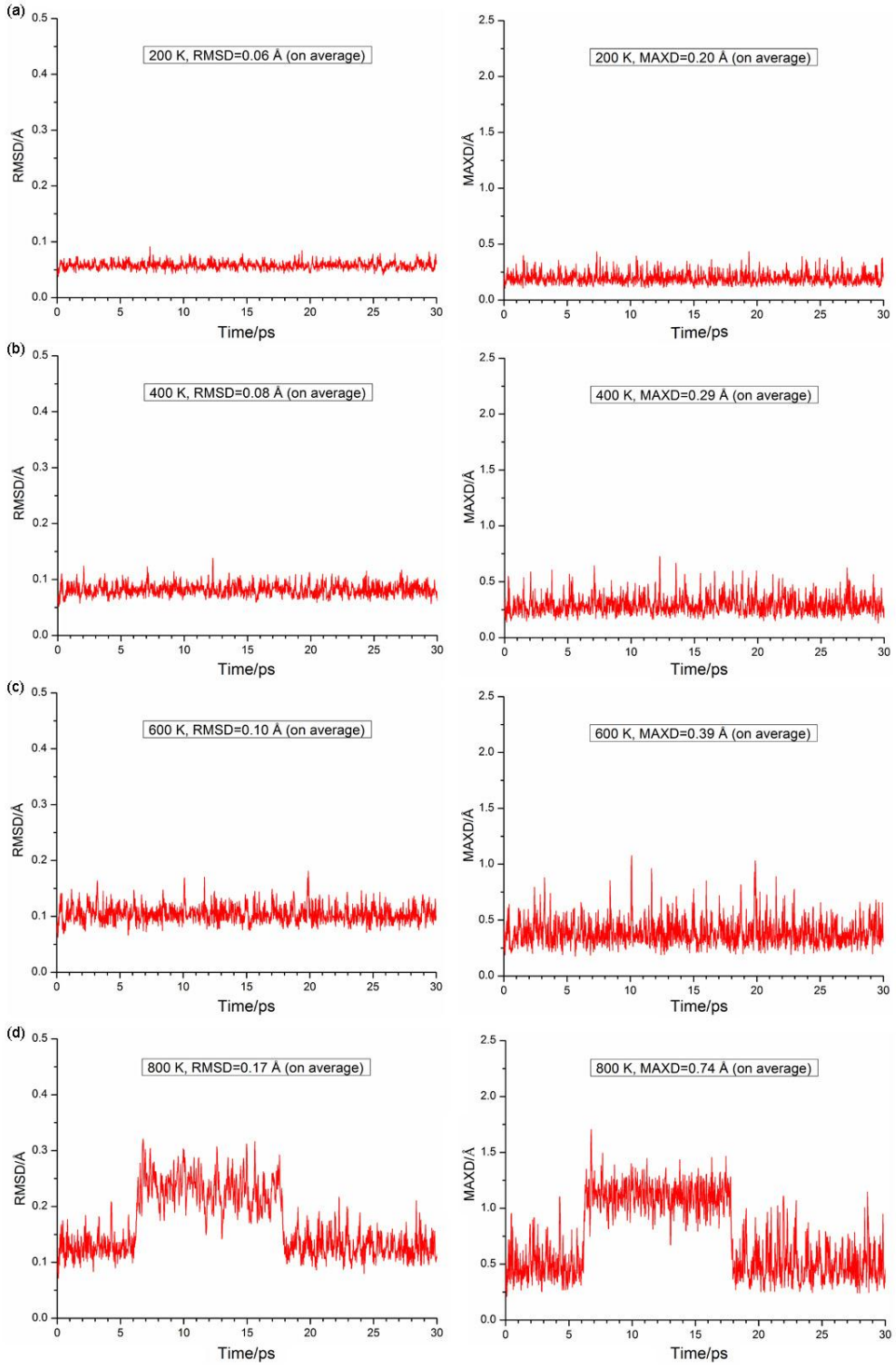

Figure S7. Born-Oppenheimer molecular dynamics simulations of C_{2v} $Li_5\&B_{36}^+$ (**3**) at (a) 200K, (b) 400K, (c) 600K and (d) 800K for 30 ps. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

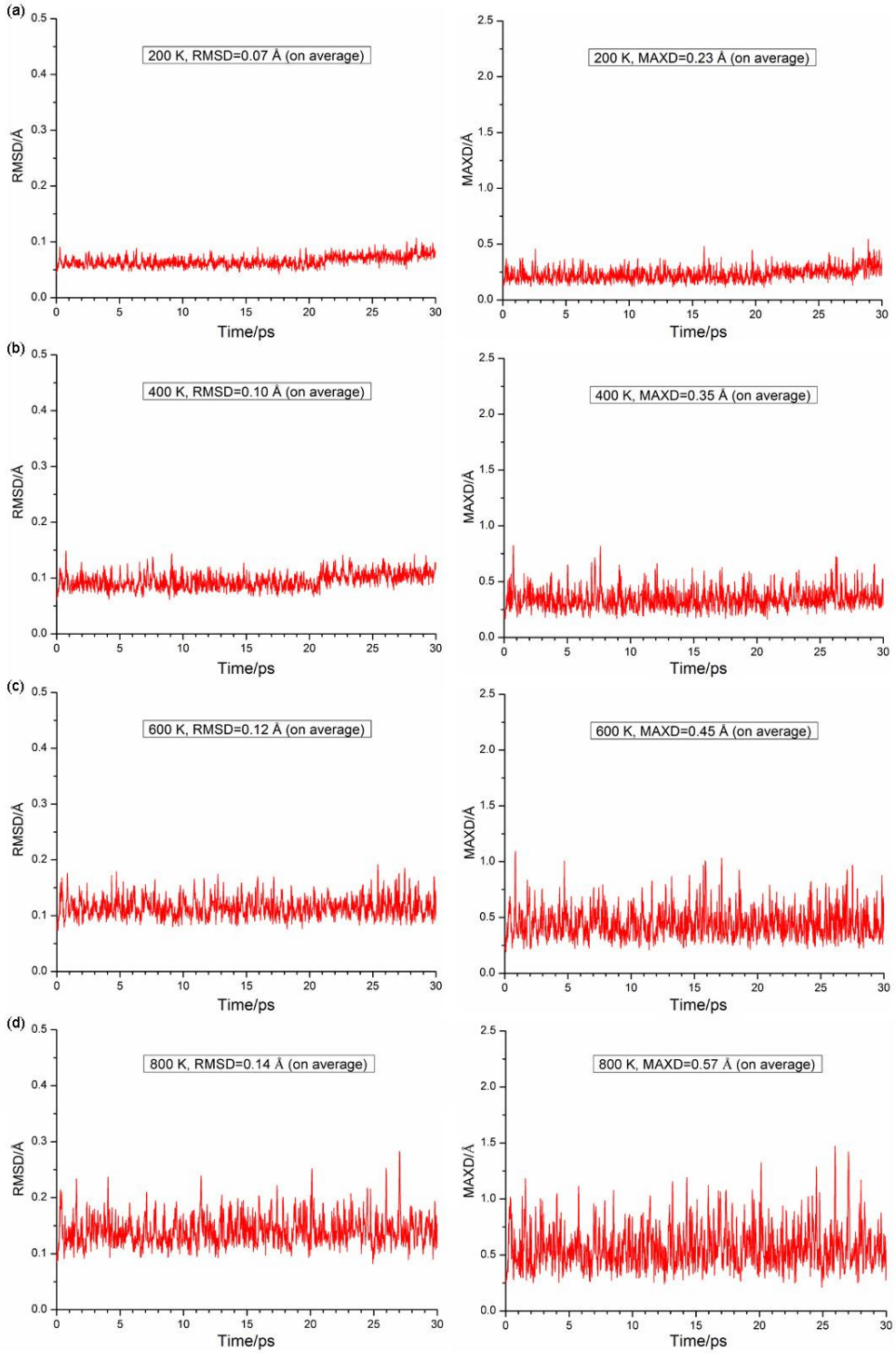

Figure S8. Born-Oppenheimer molecular dynamics simulations of T_h $Li_6\&B_{36}^{2+}$ (**4**) at (a) 200K, (b) 400K, (c) 600K and (d) 800K for 30 ps. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

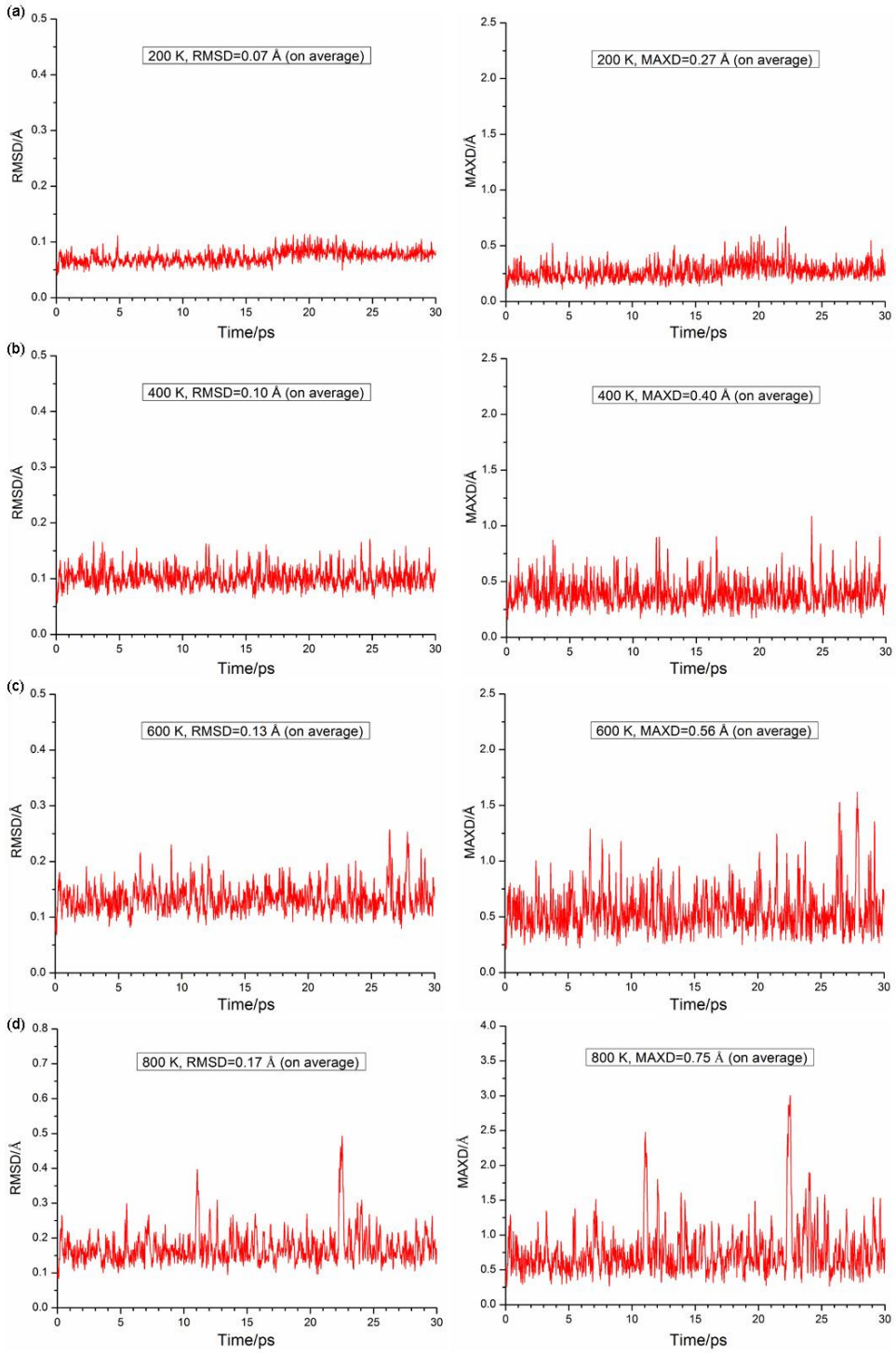

Figure S9. Simulated (a) IR and (b) Raman spectra of D_{2h} $Li_4\&B_{36}$ (**2**), C_{2v} $Li_5\&B_{36}^{+}$ (**3**), and T_h $Li_6\&B_{36}^{2+}$ (**4**) compared with that of T_h B_{36}^{4-} (**1**) at the PBE0/6-311+G* level.

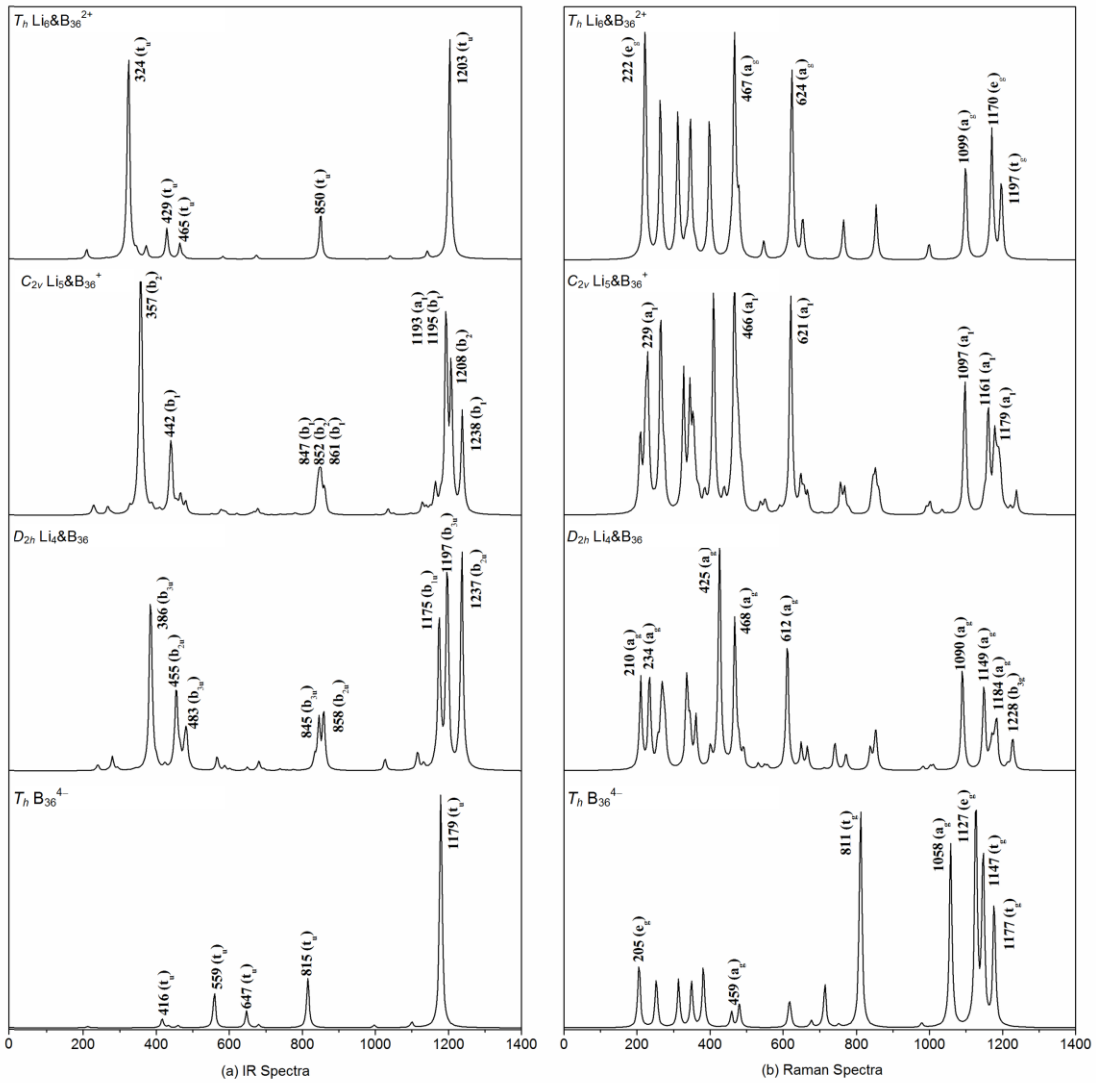

Table S1. The optimized coordinates of T_h B_{36}^{4-} (**1**), D_{2h} $Li_4\&B_{36}$ (**2**), C_{2v} $Li_5\&B_{36}^{+}$ (**3**), T_h $Li_6\&B_{36}^{2+}$ (**4**), D_{2h} $Li_2\&[Ca@B_{36}]$ (**5**), C_{2v} $Li_3\&[Ca@B_{36}]^{+}$ (**6**), and D_{2h} $Li_4\&[Ca@B_{36}]^{2+}$ (**7**) at the PBE0/6-311+G* level.

1. T_h B_{36}^{4-} (^1A_g)

B	0.00000000	1.67243500	2.65590000
B	0.00000000	-1.67243500	-2.65590000
B	-2.65590000	0.00000000	-1.67243500
B	-1.67243500	2.65590000	0.00000000
B	-0.89192500	-2.30079400	1.39659700
B	0.00000000	-1.67243500	2.65590000
B	-1.39659700	-0.89192500	-2.30079400
B	-1.39659700	0.89192500	2.30079400
B	-1.39659700	0.89192500	-2.30079400
B	-0.89192500	-2.30079400	-1.39659700
B	-0.89192500	2.30079400	1.39659700
B	-0.89192500	2.30079400	-1.39659700
B	0.00000000	1.67243500	-2.65590000
B	-2.30079400	1.39659700	-0.89192500
B	-1.67243500	-2.65590000	0.00000000
B	-1.39659700	-0.89192500	2.30079400
B	-2.30079400	1.39659700	0.89192500
B	-2.30079400	-1.39659700	-0.89192500
B	-2.65590000	0.00000000	1.67243500
B	-2.30079400	-1.39659700	0.89192500
B	2.65590000	0.00000000	-1.67243500
B	1.67243500	-2.65590000	0.00000000
B	0.89192500	2.30079400	1.39659700
B	1.39659700	0.89192500	-2.30079400
B	1.39659700	-0.89192500	2.30079400
B	1.39659700	-0.89192500	-2.30079400
B	0.89192500	2.30079400	-1.39659700
B	0.89192500	-2.30079400	1.39659700
B	0.89192500	-2.30079400	-1.39659700
B	2.30079400	-1.39659700	-0.89192500
B	1.67243500	2.65590000	0.00000000
B	1.39659700	0.89192500	2.30079400
B	2.30079400	-1.39659700	0.89192500
B	2.30079400	1.39659700	-0.89192500
B	2.65590000	0.00000000	1.67243500
B	2.30079400	1.39659700	0.89192500

2. D_{2h} $B_{36}Li_4$ (^1A_g)

B	2.64640600	1.68535300	0.00000000
B	-2.64640600	-1.68535300	0.00000000
B	-1.65829800	0.00000000	2.63479400
B	0.00000000	2.62871500	1.68725900
B	1.39121200	-2.28137100	0.88950600
B	2.64640600	-1.68535300	0.00000000
B	-2.29297900	-0.88632100	1.39761400
B	2.29297900	0.88632100	1.39761400
B	-2.29297900	0.88632100	1.39761400
B	-1.39121200	-2.28137100	0.88950600
B	1.39121200	2.28137100	0.88950600
B	-1.39121200	2.28137100	0.88950600
B	-2.64640600	1.68535300	0.00000000
B	-0.88779500	1.38535700	2.29812300
B	0.00000000	-2.62871500	1.68725900
B	2.29297900	-0.88632100	1.39761400
B	0.88779500	1.38535700	2.29812300
B	-0.88779500	-1.38535700	2.29812300
B	1.65829800	0.00000000	2.63479400
B	0.88779500	-1.38535700	2.29812300
B	-1.65829800	0.00000000	-2.63479400
B	0.00000000	-2.62871500	-1.68725900
B	1.39121200	2.28137100	-0.88950600
B	-2.29297900	0.88632100	-1.39761400
B	2.29297900	-0.88632100	-1.39761400
B	-2.29297900	-0.88632100	-1.39761400
B	-1.39121200	2.28137100	-0.88950600
B	1.39121200	-2.28137100	-0.88950600
B	-1.39121200	-2.28137100	-0.88950600
B	-0.88779500	-1.38535700	-2.29812300
B	0.00000000	2.62871500	-1.68725900
B	2.29297900	0.88632100	-1.39761400
B	0.88779500	-1.38535700	-2.29812300
B	-0.88779500	1.38535700	-2.29812300
B	1.65829800	0.00000000	-2.63479400
B	0.88779500	1.38535700	-2.29812300
Li	0.00000000	-3.92522700	0.00000000
Li	0.00000000	3.92522700	0.00000000
Li	-3.94536200	0.00000000	0.00000000
Li	3.94536200	0.00000000	0.00000000

3. C_{2v} $B_{36}Li_5^+$ ($^1A_1$)

B	-1.67724300	2.64074500	-0.05696900
B	1.67724300	-2.64074500	-0.05696900
B	0.00000000	-1.67337400	2.57793200
B	-2.64213800	0.00000000	1.62057100
B	2.29952800	1.40281800	0.82951400
B	1.67724300	2.64074500	-0.05696900
B	0.88715100	-2.28142200	1.33103700
B	-0.88715100	2.28142200	1.33103700
B	-0.88715100	-2.28142200	1.33103700
B	2.29952800	-1.40281800	0.82951400
B	-2.29952800	1.40281800	0.82951400
B	-2.29952800	-1.40281800	0.82951400
B	-1.67724300	-2.64074500	-0.05696900
B	-1.39312300	-0.88383300	2.22713800
B	2.64213800	0.00000000	1.62057100
B	0.88715100	2.28142200	1.33103700
B	-1.39312300	0.88383300	2.22713800
B	1.39312300	-0.88383300	2.22713800
B	0.00000000	1.67337400	2.57793200
B	1.39312300	0.88383300	2.22713800
B	0.00000000	-1.66405100	-2.69175500
B	2.61539200	0.00000000	-1.73574700
B	-2.26597300	1.38298400	-0.94545300
B	-0.88598000	-2.30437300	-1.46167600
B	0.88598000	2.30437300	-1.46167600
B	0.88598000	-2.30437300	-1.46167600
B	-2.26597300	-1.38298400	-0.94545300
B	2.26597300	1.38298400	-0.94545300
B	2.26597300	-1.38298400	-0.94545300
B	1.38446100	-0.89193700	-2.35870600
B	-2.61539200	0.00000000	-1.73574700
B	-0.88598000	2.30437300	-1.46167600
B	1.38446100	0.89193700	-2.35870600
B	-1.38446100	-0.89193700	-2.35870600
B	0.00000000	1.66405100	-2.69175500
B	-1.38446100	0.89193700	-2.35870600
Li	3.99465700	0.00000000	-0.07558800
Li	-3.99465700	0.00000000	-0.07558800
Li	0.00000000	-4.00889700	-0.06535100
Li	0.00000000	4.00889700	-0.06535100
Li	0.00000000	0.00000000	3.94597900

4. T_h $B_{36}Li_6^{2+}$ (^1A_g)

B	2.63385500	1.66932100	0.00000000
B	-2.63385500	-1.66932100	0.00000000
B	-1.66932100	0.00000000	2.63385500
B	0.00000000	2.63385500	1.66932100
B	1.39589400	-2.28921500	0.88724200
B	2.63385500	-1.66932100	0.00000000
B	-2.28921500	-0.88724200	1.39589400
B	2.28921500	0.88724200	1.39589400
B	-2.28921500	0.88724200	1.39589400
B	-1.39589400	-2.28921500	0.88724200
B	1.39589400	2.28921500	0.88724200
B	-1.39589400	2.28921500	0.88724200
B	-2.63385500	1.66932100	0.00000000
B	-0.88724200	1.39589400	2.28921500
B	0.00000000	-2.63385500	1.66932100
B	2.28921500	-0.88724200	1.39589400
B	0.88724200	1.39589400	2.28921500
B	-0.88724200	-1.39589400	2.28921500
B	1.66932100	0.00000000	2.63385500
B	0.88724200	-1.39589400	2.28921500
B	-1.66932100	0.00000000	-2.63385500
B	0.00000000	-2.63385500	-1.66932100
B	1.39589400	2.28921500	-0.88724200
B	-2.28921500	0.88724200	-1.39589400
B	2.28921500	-0.88724200	-1.39589400
B	-2.28921500	-0.88724200	-1.39589400
B	-1.39589400	2.28921500	-0.88724200
B	1.39589400	-2.28921500	-0.88724200
B	-1.39589400	-2.28921500	-0.88724200
B	-0.88724200	-1.39589400	-2.28921500
B	0.00000000	2.63385500	-1.66932100
B	2.28921500	0.88724200	-1.39589400
B	0.88724200	-1.39589400	-2.28921500
B	-0.88724200	1.39589400	-2.28921500
B	1.66932100	0.00000000	-2.63385500
B	0.88724200	1.39589400	-2.28921500
Li	0.00000000	0.00000000	4.07918600
Li	0.00000000	4.07918600	0.00000000
Li	0.00000000	0.00000000	-4.07918600
Li	4.07918600	0.00000000	0.00000000
Li	0.00000000	-4.07918600	0.00000000
Li	-4.07918600	0.00000000	0.00000000

5. D_{2h} Li_2&[Ca@B_{36}] (^1A_g)

B	2.64092000	0.00000000	-1.66298200
B	-2.64092000	0.00000000	1.66298200
B	-1.63319900	2.63983200	0.00000000
B	0.00000000	1.63258100	-2.62079400
B	1.41139700	0.89273400	2.30404200
B	2.64092000	0.00000000	1.66298200
B	-2.30713900	1.42082200	0.89254800
B	2.30713900	1.42082200	-0.89254800
B	-2.30713900	1.42082200	-0.89254800
B	-1.41139700	0.89273400	2.30404200
B	1.41139700	0.89273400	-2.30404200
B	-1.41139700	0.89273400	-2.30404200
B	-2.64092000	0.00000000	-1.66298200
B	-0.89102600	2.31680000	-1.41400200
B	0.00000000	1.63258100	2.62079400
B	2.30713900	1.42082200	0.89254800
B	0.89102600	2.31680000	-1.41400200
B	-0.89102600	2.31680000	1.41400200
B	1.63319900	2.63983200	0.00000000
B	0.89102600	2.31680000	1.41400200
B	-1.63319900	-2.63983200	0.00000000
B	0.00000000	-1.63258100	2.62079400
B	1.41139700	-0.89273400	-2.30404200
B	-2.30713900	-1.42082200	-0.89254800
B	2.30713900	-1.42082200	0.89254800
B	-2.30713900	-1.42082200	0.89254800
B	-1.41139700	-0.89273400	-2.30404200
B	1.41139700	-0.89273400	2.30404200
B	-1.41139700	-0.89273400	2.30404200
B	-0.89102600	-2.31680000	1.41400200
B	0.00000000	-1.63258100	-2.62079400
B	2.30713900	-1.42082200	-0.89254800
B	0.89102600	-2.31680000	1.41400200
B	-0.89102600	-2.31680000	-1.41400200
B	1.63319900	-2.63983200	0.00000000
B	0.89102600	-2.31680000	-1.41400200
Li	-3.97846600	0.00000000	0.00000000
Li	3.97846600	0.00000000	0.00000000
Ca	0.00000000	0.00000000	0.00000000

6. C_{2v} Li_3&$[Ca@B_{36}]^+$ ($^1A_1$)

B	0.00000000	2.63178200	1.70846300
B	0.00000000	-2.64887100	-1.60294400
B	2.63515600	-1.63017700	0.05328800
B	1.63171100	0.00000000	2.67277900
B	0.88972000	1.41418900	-2.23957000
B	0.00000000	2.64887100	-1.60294400
B	1.42774900	-2.31884100	-0.83382700
B	1.41541000	2.29968100	0.94778800
B	1.41541000	-2.29968100	0.94778800
B	0.88972000	-1.41418900	-2.23957000
B	0.89673400	1.41424400	2.36244000
B	0.89673400	-1.41424400	2.36244000
B	0.00000000	-2.63178200	1.70846300
B	2.32427900	-0.89040400	1.47183900
B	1.65623600	0.00000000	-2.57268100
B	1.42774900	2.31884100	-0.83382700
B	2.32427900	0.89040400	1.47183900
B	2.31073900	-0.89444600	-1.35602800
B	2.63515600	1.63017700	0.05328800
B	2.31073900	0.89444600	-1.35602800
B	-2.63515600	-1.63017700	0.05328800
B	-1.65623600	0.00000000	-2.57268100
B	-0.89673400	1.41424400	2.36244000
B	-1.41541000	-2.29968100	0.94778800
B	-1.42774900	2.31884100	-0.83382700
B	-1.42774900	-2.31884100	-0.83382700
B	-0.89673400	-1.41424400	2.36244000
B	-0.88972000	1.41418900	-2.23957000
B	-0.88972000	-1.41418900	-2.23957000
B	-2.31073900	-0.89444600	-1.35602800
B	-1.63171100	0.00000000	2.67277900
B	-1.41541000	2.29968100	0.94778800
B	-2.31073900	0.89444600	-1.35602800
B	-2.32427900	-0.89040400	1.47183900
B	-2.63515600	1.63017700	0.05328800
B	-2.32427900	0.89040400	1.47183900
Li	0.00000000	-4.04785400	0.06723000
Li	0.00000000	4.04785400	0.06723000
Ca	0.00000000	0.00000000	0.06871700
Li	0.00000000	0.00000000	-3.98416000

7. D_{2h} Li_4&$[Ca@B_{36}]^{2+}$ (^1A_g)

B	2.64297000	1.64806800	0.00000000
B	-2.64297000	-1.64806800	0.00000000
B	-1.62660900	0.00000000	2.62926400
B	0.00000000	2.62373100	1.64719200
B	1.41963100	-2.29915000	0.89317300
B	2.64297000	-1.64806800	0.00000000
B	-2.31453700	-0.88971800	1.42324800
B	2.31453700	0.88971800	1.42324800
B	-2.31453700	0.88971800	1.42324800
B	-1.41963100	-2.29915000	0.89317300
B	1.41963100	2.29915000	0.89317300
B	-1.41963100	2.29915000	0.89317300
B	-2.64297000	1.64806800	0.00000000
B	-0.89437500	1.41524600	2.31593200
B	0.00000000	-2.62373100	1.64719200
B	2.31453700	-0.88971800	1.42324800
B	0.89437500	1.41524600	2.31593200
B	-0.89437500	-1.41524600	2.31593200
B	1.62660900	0.00000000	2.62926400
B	0.89437500	-1.41524600	2.31593200
B	-1.62660900	0.00000000	-2.62926400
B	0.00000000	-2.62373100	-1.64719200
B	1.41963100	2.29915000	-0.89317300
B	-2.31453700	0.88971800	-1.42324800
B	2.31453700	-0.88971800	-1.42324800
B	-2.31453700	-0.88971800	-1.42324800
B	-1.41963100	2.29915000	-0.89317300
B	1.41963100	-2.29915000	-0.89317300
B	-1.41963100	-2.29915000	-0.89317300
B	-0.89437500	-1.41524600	-2.31593200
B	0.00000000	2.62373100	-1.64719200
B	2.31453700	0.88971800	-1.42324800
B	0.89437500	-1.41524600	-2.31593200
B	-0.89437500	1.41524600	-2.31593200
B	1.62660900	0.00000000	-2.62926400
B	0.89437500	1.41524600	-2.31593200
Li	-4.14042000	0.00000000	0.00000000
Li	4.14042000	0.00000000	0.00000000
Ca	0.00000000	0.00000000	0.00000000
Li	0.00000000	-4.12214600	0.00000000
Li	0.00000000	4.12214600	0.00000000