Supporting Information of

Does the endohedral boroshperene supersalt $FLi_2@B_{39}$ maintain "super" properties of its subunits?

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Computational details.

Geometrical structures of the endohedral superalkaliborospherenes $FLi_2@B_{39}$, related B_{39}^- nanoclusters and the superalkaline FLi_2 were obtained using density functional theory (DFT) with PBE1PBE (hereafter also termed as PBE0) hybrid functional in the ground state. Pople's 6-311+G(2d) triple-ξ quality basis set with polarization and diffused functions was employed in all cases. The adiabatic ionizations potentials (IP) and electron affinities (EA) as well as all vertical IP and EA for studied systems were obtained at the same level of theory.

The encapsulation energies of given endohedral complexes $FLi_2@B_{39}$ was calculated as the energy difference between the complex and its constituent parts:

$$\Delta E_{encap.} = E_{(FLi_2@B_{39})} - \left[E_{B_{39}} + E_{FLi_2}\right]$$

where $E_{(FLi_2@B_{39})}$, $E_{B_{39}}$ and E_{FLi_2} refer to DFT energies of complex and its fragments in equilibrium geometries. Deformation energy for each of studied complexes has been determined using following equation:

$$\Delta E_{def.} = \left[E^{complex\ geom.}_{B_{39}} - E^{eq.\ geom.}_{B_{39}}\right] + \left[E^{complex\ geom.}_{FLi_2} - E^{eq.\ geom.}_{FLi_2}\right]$$

At the same time, energy of encapsulation comprises both interaction ($\Delta E_{int.}$) and deformation ($E_{def.}$) energies. Thus $\Delta E_{int.}$ can be represented as following:

$$\Delta E_{int.} = \Delta E_{encap.} - \Delta E_{def.}$$

All calculations were carried out using Gaussian 09. Rev.D01[S1] Natural Population Analysis was carried out with NBO 6.0 program.[S2] Coupled cluster calculations were performed using the domain-based local pair natural orbital coupled cluster method with single, double, and perturbative triple excitations DLPNO-CCSD(T) with cc-PVTZ/C triple-ξ quality basis set auxiliary basis set, VeryTightSCF and Grid6 using ORCA 4.0.0.2 program[S3].

Carried out functionals and basis set benchmark revealed that adiabatic electron affinity values for SH unit could be perfectly predicted using any of the tested DFT functionals. Besides that the influence of basis set on EA is negligible. Regardless to the used basis set a relative error in predicted EA was less than 2%, whereas an absolute error value was about 0.05 to 0.07 eV. Predictions obtained for SA unit were a slightly worse. For B3LYP functional, the calculated IP values have been characterized by relative error of 11% to 12%. Very similar results were obtained for PBE0 functional – relative error is about 10% to 11%, whereas the absolute error has been determined at 0.37 to 0.40 eV level depending on the basis set. Close examination of optimized geometries for both neutral and cationic forms of the FLi_2 obtained with PBE0 and B3LYP functionals and their comparison with FLi_2 geometry obtained with CCSD/basis set has been performed (Table S2, supporting information). We found out that for doublet state of FLi_2 fragment both studied hybrid functionals reproduce perfectly bond lengths with the error less

than 1%. At the same time, inaccuracy in angle description can reach up to 9% for B3LYP and about 4% for PBE0 functional. Both functionals characterized superiorly singlet cationic state of FLi_2 with relative error level for bonds and angles description less than 0.5% regardless to the used basis set. In order to determine whether a noticeable error in the description of the IP for FLi_2 species is a consequence of geometrical inaccuracy description, we have performed calculation of IP values by both functionals for FLi_2 in geometry obtained with CCSD method. As expected, previously mentioned differences in geometries obtained by DFT and CCSD methods have had minimal effect. For both functionals, IP value differences were less than 0.01 eV. Thus, it has allowed us to assume that the main reason of the above-discussed non-negligible error in the IP prediction is most likely the well-known effect of the self-interaction error in DFT, which artificially stabilizes delocalized states.[S4-S7] The fact that the influence of this effect on B_{39} species was not observed is in a good agreement with the fact that denoted effect decreases significantly with the system size.

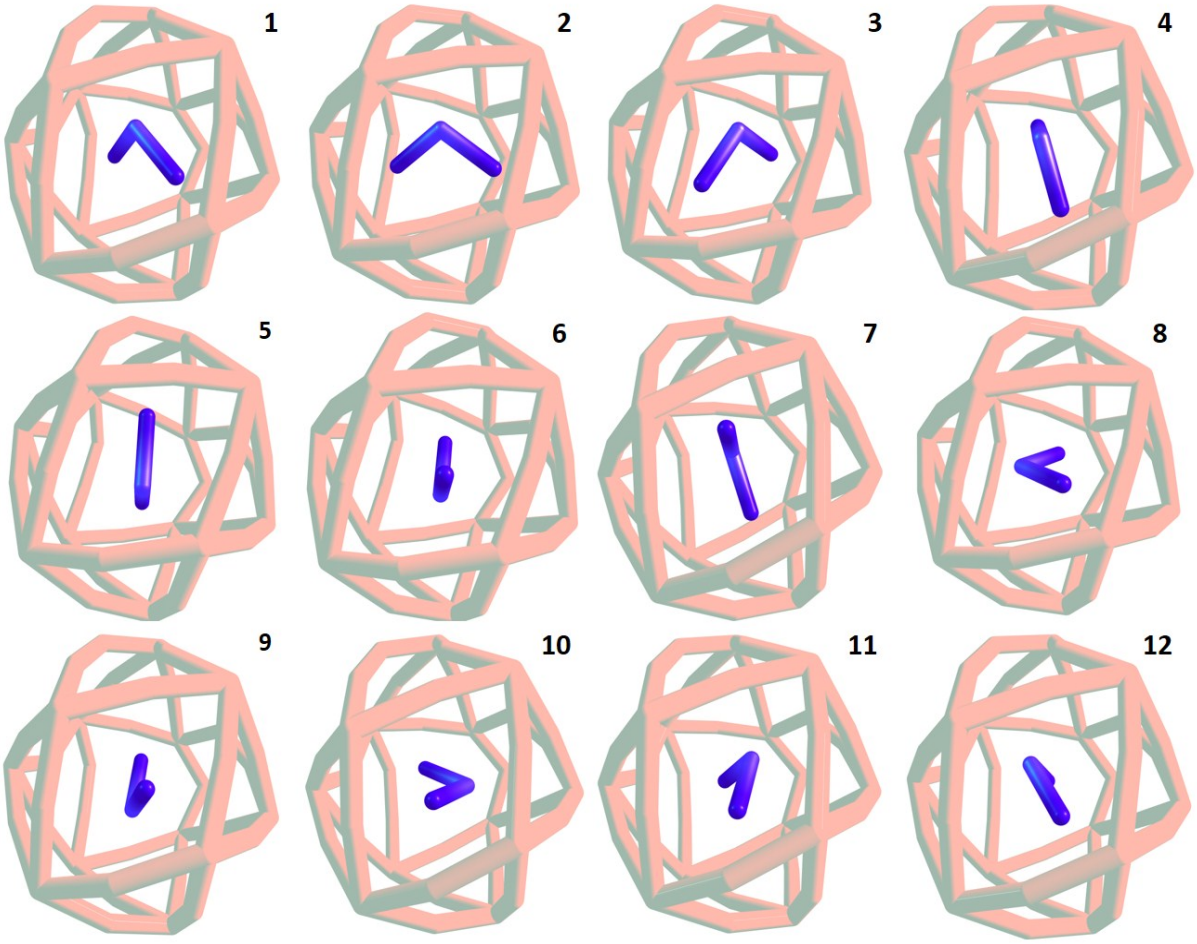


Figure S1. Initial geometries of FLi_2 subunit for free rotation verification of ^{1}(B@2) supermolecule.

Table S1. Experimentally measured and theoretically predicted at different levels of theory IP and EA values as well as statistical analysis (signed error (SE) and relative error (RE)) for FLi_2 and B_{39} species.

	B3LYP			PBE0		
	6-31+g(d)	6-311+g(d)	6-311+g(2d)	6-31+g(d)	6-311+g(d)	6-311+g(2d)
FLi_2^0, a.u	-114.9829	-115.0172	-115.0193	-114.8317	-114.8638	-114.8661
FLi_2^{1+}, a.u	-114.8274	-114.8626	-114.8639	-114.6782	-114.7113	-114.7127
Calc. IP, eV	4.23	4.21	4.23	4.18	4.15	4.17
Experim. IP value, eV	3.78±0.20					
SE, eV	0.45	0.43	0.45	0.40	0.37	0.39
RE, %	11.9	11.4	11.9	10.6	9.8	10.3

B_{39}^{1-}, a.u	-968.8544	-969.1222	-969.1476	-967.8124	-967.9327	-967.9582
B_{39}^{0}, a.u	-968.9937	-968.9818	-969.0075	-967.6694	-967.7889	-967.8147
Calc. EA, eV	3.79	3.82	3.81	3.89	3.91	3.90
Experim. EA value, eV	3.84(5)					
SE, eV	-0.05	-0.02	-0.03	0.05	0.07	0.06
RE, %	1.3	0.5	0.8	1.3	1.8	1.6

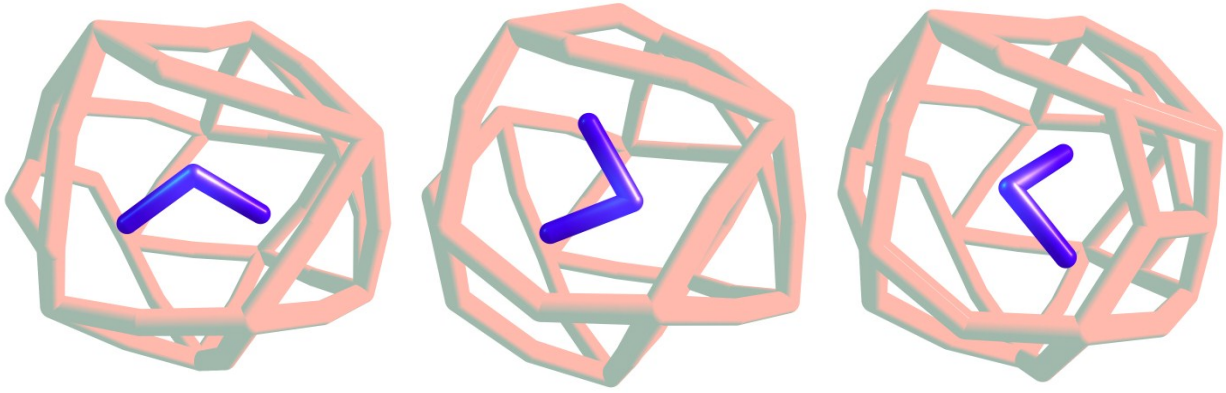
Table S2. Selected optimized geometrical parameters (bond length (d, Å) and valence angle (A, °)) and statistical analysis (absolute error (AE), mean absolute error (MAE), relative error (RE) and root-mean-squared deviation (RMSD) of atomic positions) for FLi_2 species obtained at different levels of theory.

		B3LYP			PBE0			CCSD
		6-31+g(d)	6-311+g(d)	6-311+g(2d)	6-31+g(d)	6-311+g(d)	6-311+g(2d)	6-311+g(2d)
{0,2}	d(F^1Li), Å	1.6824	1.6821	1.6756	1.6848	1.6859	1.6785	1.6901
	A(F^1LiF^2), °	110.445	109.949	107.937	105.378	105.031	103.831	101.010
	MAE, Å d(FLi)	0.0077	0.008	0.0145	0.0053	0.0048	0.0116	
	RE, % d(FLi)	0.46	0.47	0.86	0.31	0.28	0.69	
	AE, ° A(F^1LiF^2)	9.435	8.504	6.492	3.933	3.586	2.386	
	RE, % A(F^1LiF^2)	9.34	8.42	6.43	3.89	3.55	2.36	
	RMSD[a]	0.059			0.023			
{1,1}	d(F^1Li), Å	1.6774	1.6759	1.6694	1.6754	1.6752	1.6685	1.6809
	A(F^1LiF^2), °	173.844	173.876	174.011	173.887	173.890	174.03	173.734
	MAE, Å d(FLi)	0.0035	0.0050	0.0115	0.0056	0.0057	0.0124	
	RE, % d(FLi)	0.21	0.30	0.68	0.33	0.34	0.74	
	AE, ° A(F^1LiF^2)	0.110	0.142	0.277	0.153	0.156	0.296	
	RE, % A(F^1LiF^2)	0.06	0.08	0.16	0.09	0.09	0.17	
	RMSD[a]	0.009			0.010			

[a] RMSD was minimized for all atoms of FLi_2 for geometries obtained with B3LYP or PBE0 functionals and CCSD method with 6-311+g(2d) basis set using Chemcraft software v. 1.80[S8]

Figure S2. Graphical representation and Relative energies of ^{3}(A@1), ^{2}(B@1)$^{+}$, ^{2}(A@2)$^{-}$ and ^{1}(B@2) supermolecules conformers obtained at PBE0/6-31+G(d) level of theory.

A. Graphical representation and relative energies of ^{3}(A@1) conformers

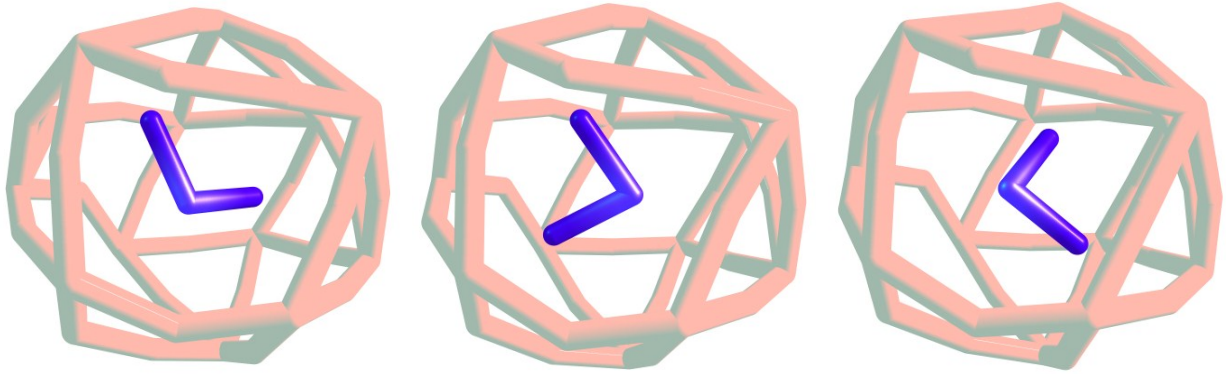


^{3}(A@1) Conf. 1
E_{rel} = 0.0 kcal/mol

^{3}(A@1) Conf. 2
E_{rel} = 4.3 kcal/mol

^{3}(A@1) Conf. 3
E_{rel} = 20.6 kcal/mol

B. Graphical representation and relative energies of ^{2}(B@1)$^{+}$ conformers

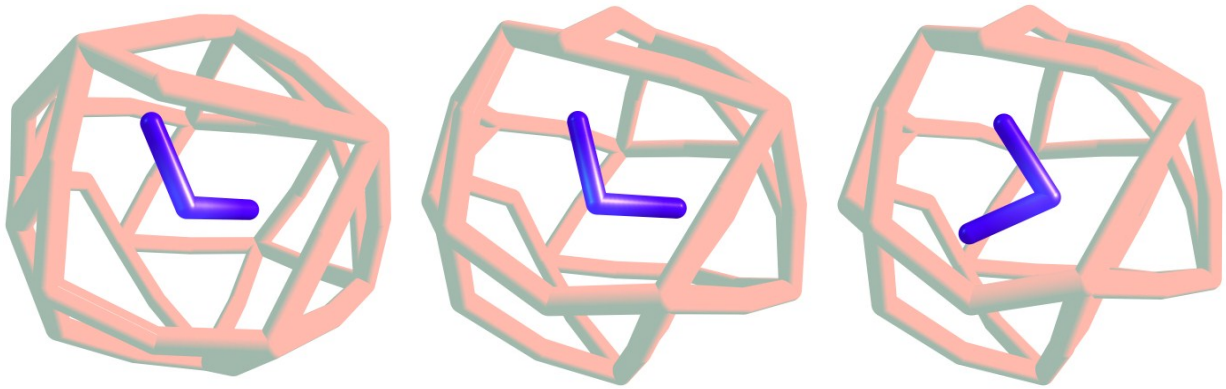


^{2}(B@1)$^{+}$ Conf. 1
E_{rel} = 0.0 kcal/mol

^{2}(B@1)$^{+}$ Conf. 2
E_{rel} = 6.7 kcal/mol

^{2}(B@1)$^{+}$ Conf. 3
E_{rel} = 19.0 kcal/mol

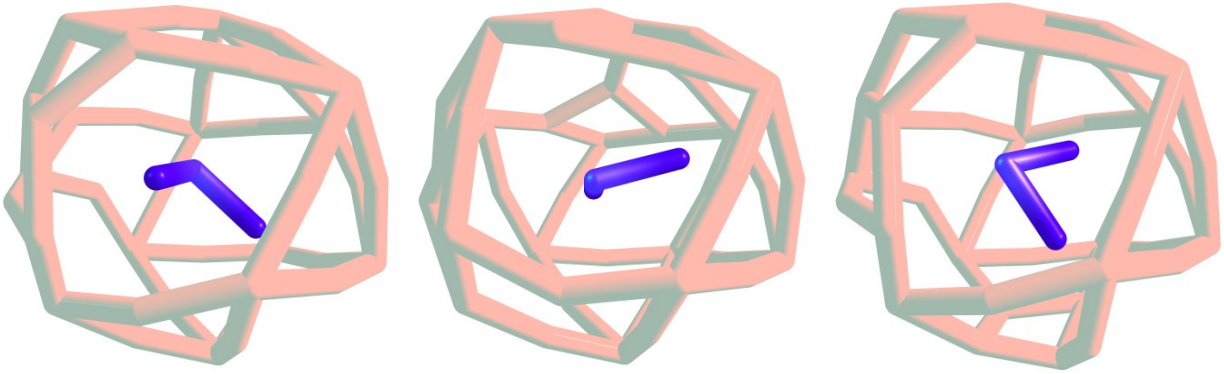
C. Graphical representation and relative energies of ^{2}(A@2)$^{-}$ conformers



^{2}(A@2)$^{-}$ Conf. 1
E_{rel} = 0.0 kcal/mol

^{2}(A@2)$^{-}$ Conf. 2
E_{rel} = 0.4 kcal/mol

^{2}(A@2)$^{-}$ Conf. 3
E_{rel} = 5.8 kcal/mol



^{2}(A@2)$^-$ Conf. 4
E_{rel} = 7.4 kcal/mol

^{2}(A@2)$^-$ Conf. 5
E_{rel} = 20.6 kcal/mol

^{2}(A@2)$^-$ Conf. 6
E_{rel} = 23.8 kcal/mol

Table S3. Encapsulation energies determined in the manner indicated at Scheme S1 for various hybrid functionals with 6-31+g(d) basis set applied for supermolecules of interest.

	B3LYP	PBE0	TPSSh	mPW1PW91	HSE06
^{3}(A@1), kcal/mol	3.17	-14.21	-17.37	-9.52	-12.28
^{2}(B@1)$^+$, kcal/mol	33.27	19.41	17.21	24.18	20.69
^{2}(A@2)$^-$, kcal/mol	2.49	-14.67	-17.09	-10.08	-13.27
^{1}(B@2), kcal/mol	-42.87	-56.14	-58.39	-51.34	-54.87

Table S4. Root-mean-squared deviation (RMSD[a]) of atomic positions for studied with different functionals ^{3}(A@1), ^{2}(B@1)$^+$, ^{2}(A@2)$^-$ and ^{1}(B@2) supermolecules optimized at PBE0/6-31+G(d) level of theory.

	B3LYP	PBE0	TPSSh	mPW1PW91	HSE06
	^{3}(A@1)				
B3LYP	0	0.02286	0.02667	0.01985	0.02207
PBE0		0	0.01287	0.00400	0.00391
TPSSh			0	0.01421	0.01305
mPW1PW91				0	0.00627
HSE06					0
	^{2}(B@1)$^+$				
B3LYP	0	0.02073	0.02212	0.01885	0.01560
PBE0		0	0.00928	0.00281	0.00906
TPSSh			0	0.00950	0.01320
mPW1PW91				0	0.00829
HSE06					0

	^{2}(A@2)$^-$				
B3LYP	0	0.01989	0.01956	0.01809	0.01867
PBE0		0	0.00929	0.00262	0.00329
TPSSh			0	0.00907	0.00995
mPW1PW91				0	0.00449
HSE06					0
	^{1}(B@2)				
B3LYP	0	0.02072	0.02112	0.01829	0.02042
PBE0		0	0.00882	0.00310	0.00292
TPSSh			0	0.00905	0.00966
mPW1PW91				0	0.00488
HSE06					0

[a] RMSD was minimized for all atoms for geometries obtained with denoted functionals with 6-31+g(d) basis set using Chemcraft software v. 1.80

Table S5. Comparison of geometries of free FLi_2 molecule and FLi_2 encapsulated in $FLi_2@B_{39}$ systems obtained at PBE0/6-311+g(2d) level of theory.

		FLi2	^{3}(A@1)	^{2}(B@1)$^+$	^{2}(A@2)$^-$	^{1}(B@2)
{0,2}	B, Å	1.67853	1.60435	-	1.60249	-
	A, °	103.831	107.499	-	105.333	-
{1,1}	B, Å	1.66850	-	1.61400	-	1.59513
	A, °	174.030	-	103.284	-	104.582

Table S6. Charges and spin density analysis performed with natural population analysis scheme.

	^{3}(A@1)		^{2}(B@1)$^+$		^{2}(A@2)$^-$		^{1}(B@2)	
	Charge	Spin	Charge	Spin	Charge	Spin	Charge	Spin
Frag. 1	-0.849	1.998	0.176	0.998	-1.836	0.999	-0.833	0.000
Frag. 2	0.849	0.002	0.824	0.002	0.836	0.001	0.833	0.000
Total	0.000	2.000	1.000	1.000	-1.000	1.000	0.000	0.000
q(Li^1)	0.821	0.001	0.816	0.000	0.819	0.001	0.821	0.000
q(Li^2)	0.845	0.000	0.841	0.000	0.845	0.000	0.845	0.000
q(F)	-0.816	0.001	-0.833	0.002	-0.828	0.000	-0.833	0.000

Table S7. Computationally obtained values of adiabatic IP and EA, vertical IP, AE, EA and DE energies for B_{39}, FLi_2 species and ^{1}(B@2) endohedral complex, as well as statistical analysis (signed error (SE) and relative error values for the denoted species.

	^{1}(B@2)	B_{39} {0,2}	FLi_2 {0,2}
Adiabatic IP, eV	7.19	-	4.17
Vertical IP, eV	7.34	-	4.86
Vertical AE, eV	6.99	-	4.04
SE(AIP-VIP) , eV	-0.15	-	-0.69
RE, %	2.1	-	16.6
SE(AIP-VAE) , eV	0.20	-	0.13
RE, %	2.8	-	3.1
Adiabatic EA, eV	2.38	3.90	-
Vertical EA, eV	2.20	3.77	-
Vertical DE, eV	2.54	4.03	-
SE(AEA-VEA) , eV	0.18	0.13	-
RE, %	7.6	3.3	-
SE(AEA-VDE) , eV	-0.16	0.13	-
RE, %	6.7	3.3	-

Scheme S1. Method for calculation of encapsulation ($\Delta E_{encap.}$), deformation ($\Delta E_{def.}$) and interaction ($\Delta E_{int.}$) energies for studied supermolecules.[a]

$$\underset{\text{Individual}}{B_{39}^{X_1,Y_1} + FLi_2^{X_2,Y_2}} \rightarrow \underset{\text{Complex}}{(FLi_2@B_{39})^{X_3,Y_3}}$$

$$\Delta E_{encap.} = E(FLi_2@B_{39})^{X_3,Y_3} - (E_{B_{39}^{X_1,Y_1}}^{idivid.} + E_{FLi_2^{X_2,Y_2}}^{idivid.}) = \Delta E_{def.} + \Delta E_{int.}$$

$$\Delta E_{def.} = (E_{B_{39}^{X_1,Y_1}}^{complex\ geom.} - E_{B_{39}^{X_1,Y_1}}^{eq.geom.}) + (E_{FLi_2^{X_2,Y_2}}^{complex\ geom.} - E_{FLi_2^{X_2,Y_2}}^{eq.geom.})$$

Encapsulation energy:

$$^3(\text{A@1}) = E(FLi_2@B_{39})^{0,3} - (E_{B_{39}^{0,2}}^{idivid.} + E_{FLi_2^{0,2}}^{idivid.}) \quad \textbf{(E.1)}$$

$$^2(\text{B@1})^+ = E(FLi_2@B_{39})^{1,2} - (E_{B_{39}^{0,2}}^{idivid.} + E_{FLi_2^{1,1}}^{idivid.}) \quad \textbf{(E.2)}$$

$$^2(\text{A@2})^- = E(FLi_2@B_{39})^{-1,2} - (E_{B_{39}^{-1,1}}^{idivid.} + E_{FLi_2^{0,2}}^{idivid.}) \quad \textbf{(E.3)}$$

$$^1(\text{B@2}) = E(FLi_2@B_{39})^{0,1} - (E_{B_{39}^{-1,1}}^{idivid.} + E_{FLi_2^{1,1}}^{idivid.}) \quad \textbf{(E.4)}$$

Deformation energy:

Fragment 1 (**F1**) Fragment 2 (**F2**)

$$^3(\text{A@1}) = (E_{B_{39}^{0,2}}^{complex\ geom.} - E_{B_{39}^{0,2}}^{eq.geom.}) + (E_{FLi_2^{0,2}}^{complex\ geom.} - E_{FLi_2^{0,2}}^{eq.geom.}) \quad \textbf{(D.1)}$$

$$^2(\text{B@1})^+ = (E_{B_{39}^{0,2}}^{complex\ geom.} - E_{B_{39}^{0,2}}^{eq.geom.}) + (E_{FLi_2^{1,1}}^{complex\ geom.} - E_{FLi_2^{1,1}}^{eq.geom.}) \quad \textbf{(D.2)}$$

$$^2(\text{A@2})^- = (E_{B_{39}^{-1,1}}^{complex\ geom.} - E_{B_{39}^{-1,1}}^{eq.geom.}) + (E_{FLi_2^{0,2}}^{complex\ geom.} - E_{FLi_2^{0,2}}^{eq.geom.}) \quad \textbf{(D.3)}$$

$$^1(\text{B@2}) = (E_{B_{39}^{-1,1}}^{complex\ geom.} - E_{B_{39}^{-1,1}}^{eq.geom.}) + (E_{FLi_2^{1,1}}^{complex\ geom.} - E_{FLi_2^{1,1}}^{eq.geom.}) \quad \textbf{(D.4)}$$

[a] X_i, Y_i charge and multiplicity for denoted species.

Cartesian coordinates for studied molecules.

^{1}(B@2). Initial geometry 1.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	0.8235253	-1.1920088	-0.5834768
Li	-0.8901713	0.0664656	0.8123548
F	0.4395780	0.2729991	-0.0672329

^{1}(B@2). Initial geometry 2.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	-1.0742112
B	0.8944390	-2.5253050	1.3098481
B	-1.1919380	-2.3111180	-0.073991
B	2.0753630	2.2951180	0.9193270
B	-0.5151740	2.8261740	-1.4310370
B	-2.7913240	-0.1524600	1.3058420
B	-0.8961000	0.0044470	-1.0507580
B	2.8944110	-1.0705780	-0.0405680
B	-0.2141380	-1.3804670	-1.8627840
B	0.2475010	-0.0182730	3.0548490
B	1.4161140	-0.9278650	1.4058360
B	2.9846400	0.8702570	2.4524380
B	0.5544900	2.5487410	-3.0630130
B	-3.0671690	-0.1883940	-2.4215780
B	-1.0557490	2.6076150	-0.7749930
B	2.8571470	-0.4088930	-1.5063470
B	-1.8006990	-2.3792630	1.0370200
B	-0.7115580	-2.7448870	-1.5919910
B	-0.2185720	-1.4549610	-1.7746780
B	-2.9818350	-1.0631010	-0.3333360
B	-1.3262570	-0.0959930	-1.5075150
B	3.1684590	-0.8355090	-2.4422780
B	2.3732730	-1.8690820	-0.5334410
B	-0.3583070	1.3558570	-2.5936640
B	-2.0360280	1.3154070	-0.1941230
B	-2.0204900	0.7363940	-1.3716770
B	1.4853580	-1.5541080	-2.4155000
B	-0.1180350	-2.8648970	-1.7989340
B	-3.1139450	0.7216480	2.1277630
B	0.4183390	-2.6229060	2.1840160
B	0.0320040	2.7393620	0.0320650
B	-2.9151870	1.4428740	-0.5132660
B	-1.5069310	2.2174110	1.5726860
B	2.9942290	0.5393030	1.4995420
B	2.2147420	-0.0285680	0.9365020
B	0.7029000	0.1278880	1.2883580
B	2.7012430	2.0219680	0.9763880
B	-0.3729360	1.4124100	2.4041540
B	1.1643040	2.6514700	2.9196990
Li	0.2183715	-0.9458737	0.3808090
Li	-0.2526025	-0.1953373	2.3535780
F	0.4071629	0.2886670	0.3490230

^{1}(B@2). Initial geometry 3.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	-0.9131726	-0.3218561	-0.7470471
Li	0.8747393	-0.8147442	0.9934392
F	0.4113652	0.2840563	-0.0847471

^{1}(B@2). Initial geometry 4.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	-1.0905549	-0.7262039	0.2729601
Li	1.4217568	-0.4749200	-0.0336449
F	0.0417301	0.3485800	-0.0776702

^{1}(B@2). Initial geometry 5.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	0.1810751	-1.5716354	0.2957859
Li	0.7045984	0.8672230	-0.2009570
F	-0.5127415	-0.1481316	0.0668161

^{1}(B@2). Initial geometry 6.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	1.3931423	-0.6143947	0.0364726
Li	-0.8336948	0.6138137	-0.0030286
F	-0.1865155	-0.8519630	0.1282010

^{1}(B@2). Initial geometry 7.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	0.0551788	1.0099198	-0.1456199
Li	-0.4434801	-1.4458593	0.2895218
F	0.7612333	-0.4166044	0.0177431

^{1}(B@2). Initial geometry 8.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	-0.9611751	0.3864994	0.3558513
Li	1.2538178	-0.8629402	0.3954373
F	0.0802893	-0.3761032	-0.5896436

^{1}(B@2). Initial geometry 9.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	-0.8318562	0.6120463	0.0962919
Li	1.3910825	-0.6229550	0.1429326
F	-0.1862942	-0.8416352	-0.0775795

^{1}(B@2). Initial geometry 10.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	-0.9506460	0.4008168	-0.2535648
Li	1.2645026	-0.8487784	-0.2756650
F	0.0590754	-0.4045824	0.6908748

^{1}(B@2). Initial geometry 11.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	1.0936308	-1.1372276	-0.1741715
Li	-1.1161701	0.1200832	-0.1048198
F	0.3954713	0.1646003	0.4406364

^{1}(B@2). Initial geometry 12.

Atom	X	Y	Z
B	-2.6897320	-1.7700300	0.9193270
B	0.8944390	-2.5253050	-1.4310370
B	-1.1919380	-2.3111180	1.3058420
B	2.0753630	2.2951180	-1.0507580
B	-0.5151740	2.8261740	-0.0405680
B	-2.7913240	-0.1524600	-1.8627840
B	-0.8961000	0.0044470	3.0548490
B	2.8944110	-1.0705780	1.4058360
B	-0.2141380	-1.3804670	2.4524380
B	0.2475010	-0.0182730	-3.0630130
B	1.4161140	-0.9278650	-2.4215780
B	2.9846400	0.8702570	-0.7749930
B	0.5544900	2.5487410	-1.5063470
B	-3.0671690	-0.1883940	1.0370200
B	-1.0557490	2.6076150	-1.5919910
B	2.8571470	-0.4088930	-1.7746780
B	-1.8006990	-2.3792630	-0.3333360
B	-0.7115580	-2.7448870	-1.5075150
B	-0.2185720	-1.4549610	-2.4422780
B	-2.9818350	-1.0631010	-0.5334410
B	-1.3262570	-0.0959930	-2.5936640
B	3.1684590	-0.8355090	-0.1941230
B	2.3732730	-1.8690820	-1.3716770
B	-0.3583070	1.3558570	-2.4155000
B	-2.0360280	1.3154070	-1.7989340
B	-2.0204900	0.7363940	2.1277630
B	1.4853580	-1.5541080	2.1840160
B	-0.1180350	-2.8648970	0.0320650
B	-3.1139450	0.7216480	-0.5132660
B	0.4183390	-2.6229060	1.5726860
B	0.0320040	2.7393620	1.4995420
B	-2.9151870	1.4428740	0.9365020
B	-1.5069310	2.2174110	1.2883580
B	2.9942290	0.5393030	0.9763880
B	2.2147420	-0.0285680	2.4041540
B	0.7029000	0.1278880	2.9196990
B	2.7012430	2.0219680	0.3808090
B	-0.3729360	1.4124100	2.3535780
B	1.1643040	2.6514700	0.3490230
Li	1.0964720	-1.1522860	0.1973192
Li	-1.1106362	0.1094718	0.2714869
F	0.3870961	0.1902702	-0.3071611

^{1}(B@2) Conformer 1.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.68592500	-1.7678940	0.9354790
B	0.87978000	-2.5232180	-1.4430310
B	-1.18627300	-2.3120990	1.3102530
B	2.07193100	2.2942480	-1.0615300
B	-0.51122700	2.8277860	-0.0313310
B	-2.80498300	-0.1444030	-1.8425100
B	-0.87417100	-0.0007230	3.0615860
B	2.90278700	-1.0782720	1.3825530
B	-0.19910300	-1.3854720	2.4516040
B	0.22486600	-0.0118810	-3.0662260
B	1.39743100	-0.9226830	-2.4339180
B	2.98048900	0.8668810	-0.7952850
B	0.54801400	2.5507500	-1.5054240
B	-3.06022800	-0.1857570	1.0590530
B	-1.06295900	2.6129450	-1.5791750
B	2.84554300	-0.4102180	-1.7967760
B	-1.80707200	-2.3754510	-0.3248650
B	-0.72674800	-2.7397030	-1.5071470
B	-0.23797800	-1.4486040	-2.4426730
B	-2.98814900	-1.0573480	-0.5134060
B	-1.34525100	-0.0883260	-2.5842710
B	3.16441700	-0.8396440	-0.2184560
B	2.35986900	-1.8696100	-1.3932980
B	-0.37387900	1.3614530	-2.4101070
B	-2.04686200	1.3225350	-1.7807870
B	-2.00383000	0.7352580	2.1441110
B	1.49813100	-1.5602760	2.1700980
B	-0.12189700	-2.8640990	0.0277800
B	-3.11676000	0.7274340	-0.4888940
B	0.42555500	-2.6274350	1.5650280
B	0.04778100	2.7354170	1.5040790
B	-2.90608000	1.4455230	0.9609180
B	-1.49340400	2.2162840	1.3032490
B	3.00182500	0.5329370	0.9561970
B	2.23252800	-0.0373280	2.3882250
B	0.72423200	0.1194860	2.9141700
B	2.70741500	2.0169500	0.3649760
B	-0.35308300	1.4075610	2.3585460
B	1.17114900	2.6485910	0.3449230
Li	1.11609500	-1.1331600	0.1700520
Li	-1.16044300	-0.0093680	0.0508600
F	0.41625000	0.2860720	-0.0645710

^{1}(B@2) Conformer 2.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.7248360	-1.8088340	0.9153850
B	0.8530680	-2.5581800	-1.3819130
B	-1.2437790	-2.3397430	1.3313170
B	2.0608360	2.3461850	-1.0292750
B	-0.5293360	2.8352420	-0.0261850
B	-2.8079270	-0.1212400	-1.8524560
B	-0.9373420	-0.0260050	3.1118540
B	2.8090550	-1.1036870	1.4320220
B	-0.2621800	-1.4267170	2.5049410
B	0.2282100	-0.0031880	-3.0576510
B	1.4027090	-0.9524630	-2.4747810
B	2.9770510	0.8832570	-0.7415850
B	0.5503050	2.6221070	-1.5394760
B	-2.9882230	-0.2110550	1.0322010
B	-1.0660260	2.6253510	-1.5976410
B	2.7863400	-0.3910200	-1.7445010
B	-1.8329760	-2.4152730	-0.3080140
B	-0.7387920	-2.7501980	-1.4847920
B	-0.2338480	-1.4569990	-2.4212130
B	-2.9020630	-1.0452360	-0.5230480
B	-1.3470630	-0.0804450	-2.5473260
B	3.0674160	-0.8247500	-0.1577320
B	2.2957410	-1.8555510	-1.3297570
B	-0.4092260	1.4231030	-2.5234870
B	-2.0574400	1.3298850	-1.8235070
B	-2.0445710	0.7193400	2.1649910
B	1.4329940	-1.6202860	2.2319360
B	-0.1633000	-2.9173740	0.0661900
B	-3.0050830	0.7249620	-0.4643580
B	0.3580590	-2.6797640	1.6215890
B	0.0188370	2.6825200	1.5052010
B	-2.9445780	1.4210640	0.9967150
B	-1.5132530	2.1391630	1.2698790
B	2.9304120	0.5060220	1.0161030
B	2.1349900	-0.0641590	2.4356290
B	0.6504550	0.0987630	3.0037370
B	2.6198390	1.9971210	0.4292000
B	-0.3875880	1.3598920	2.3745840
B	1.1327630	2.7177420	0.3495830
Li	0.9084810	-1.1085560	0.2965560
Li	0.8039360	0.5994520	-1.0267820
F	-0.2322790	0.0446940	0.1059260

^{1}(B@2) Conformer 3.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6725890	-1.8260930	0.8980560
B	0.9095080	-2.5659910	-1.3905520
B	-1.1770370	-2.3437690	1.3140080
B	2.0506790	2.1848860	-1.0365300
B	-0.5159990	2.9286510	-0.0303130
B	-2.8149260	-0.1590570	-1.8886920
B	-0.8701780	-0.0267240	3.0481720
B	2.9432500	-1.1294090	1.4034220
B	-0.1828750	-1.4201180	2.4457960
B	0.2524370	-0.0321740	-3.0211420
B	1.4312470	-0.9443800	-2.4055070
B	3.0424250	0.8234620	-0.7463140
B	0.5396610	2.4910690	-1.4787340
B	-2.9492130	-0.2242710	1.0027820
B	-1.0869050	2.5935230	-1.5789840
B	2.8671730	-0.4367450	-1.7524870
B	-1.7802630	-2.4271190	-0.3368960
B	-0.6823840	-2.7929630	-1.4973630
B	-0.2068930	-1.4695130	-2.3853050
B	-2.9096730	-1.0817570	-0.5386270
B	-1.3383320	-0.1142590	-2.5947680
B	3.2630290	-0.8847400	-0.1959280
B	2.3671500	-1.8894800	-1.3197100
B	-0.3931250	1.3513950	-2.4367010
B	-2.1087710	1.3238690	-1.9000880
B	-2.0081110	0.7342250	2.1464560
B	1.5041260	-1.6099150	2.1090360
B	-0.0816230	-2.8661330	0.0407940
B	-3.1030620	0.7008780	-0.5185830
B	0.4221400	-2.6803800	1.5880850
B	0.0330560	2.7188250	1.5047270
B	-2.9029860	1.4278680	0.9451740
B	-1.5427420	2.2502390	1.3638060
B	3.0948920	0.4804330	1.0022530
B	2.2198320	-0.0708190	2.3663620
B	0.7202280	0.1237420	2.8944720
B	2.6387610	1.9274850	0.4232300
B	-0.3762860	1.4065960	2.3895000
B	1.1441040	2.6574980	0.3271380
Li	-1.0773560	0.9749500	-0.1658480
Li	1.2693960	-0.4608310	0.1064450
F	-0.2819820	-0.3278120	0.0394170

^{1}(B@2) Conformer 4.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6420680	-1.8198690	0.9233050
B	0.8847620	-2.5378520	-1.3491370
B	-1.2006320	-2.4580650	1.3545580
B	2.1239460	2.2786630	-1.0531150
B	-0.4634710	2.9718240	-0.0292290
B	-2.7648470	-0.1607160	-1.8802660
B	-0.8537390	-0.0206320	3.0413230
B	2.9403930	-1.0940510	1.4260750
B	-0.2181810	-1.4291350	2.4259650
B	0.2764310	-0.0422590	-3.0220380
B	1.4153850	-0.9592090	-2.3449890
B	2.9809220	0.8259220	-0.7770220
B	0.5951830	2.5343940	-1.4815950
B	-2.9077800	-0.2025280	1.0060200
B	-1.0317310	2.6070260	-1.5760130
B	2.8751830	-0.4673480	-1.7489900
B	-1.8492510	-2.5635460	-0.3125120
B	-0.7226380	-2.7986780	-1.4794190
B	-0.2043740	-1.4989030	-2.4141290
B	-2.8438780	-1.0789200	-0.5369700
B	-1.2967140	-0.1140390	-2.5826690
B	3.1180270	-0.8610290	-0.1627130
B	2.3613690	-1.8987840	-1.2947890
B	-0.3417630	1.3619040	-2.4365930
B	-2.0297390	1.3220690	-1.8691370
B	-1.9512180	0.7536170	2.1290370
B	1.4654170	-1.5313950	2.0500060
B	-0.1191030	-3.0362820	0.0456800
B	-3.0007280	0.6982760	-0.5048160
B	0.4229550	-2.6758740	1.5484920
B	0.0831380	2.7456990	1.5090500
B	-2.8404890	1.4492040	0.9345040
B	-1.4836500	2.2776400	1.3489020
B	3.0084540	0.5169470	0.9892890
B	2.2563730	-0.0626880	2.4075420
B	0.7374270	0.0805080	2.8790480
B	2.7307810	1.9967870	0.3806390
B	-0.3414360	1.4212050	2.3940120
B	1.2002780	2.6719570	0.3273900
Li	-0.8261730	0.9775590	-0.1367230
Li	-0.4712310	-1.0349370	-0.0415320
F	0.5781930	0.1706800	0.0536200

^{3}(A@1) Conformer 1.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6987660	-1.8033920	1.0059200
B	0.8850420	-2.5644400	-1.3845800
B	-1.2058630	-2.3632980	1.4149560
B	2.1009620	2.3191710	-1.1081310
B	-0.6000820	2.8435230	-0.0442670
B	-2.7744520	-0.2006490	-1.7943360
B	-0.8824530	-0.0064970	3.1092270
B	2.9665470	-1.1260470	1.4235250
B	-0.2289780	-1.4180810	2.5092200
B	0.2454640	-0.0710850	-3.0381860
B	1.4615670	-1.0019450	-2.4877160
B	3.1204960	0.8391230	-0.7941190
B	0.5608230	2.5098020	-1.5012980
B	-3.0781670	-0.2110320	1.1137370
B	-1.0982590	2.6122140	-1.5990240
B	2.8845340	-0.4735780	-1.7635870
B	-1.8036350	-2.3604360	-0.2660020
B	-0.7058000	-2.7551400	-1.4217990
B	-0.1819700	-1.4950510	-2.3554180
B	-2.9688060	-1.0730190	-0.4411790
B	-1.3216510	-0.1493840	-2.5740580
B	3.1256750	-0.9417300	-0.1728060
B	2.3579430	-1.9151430	-1.3384510
B	-0.3852860	1.3585020	-2.4083530
B	-2.0125300	1.2529010	-1.6909300
B	-2.0260840	0.7457530	2.2230350
B	1.4209020	-1.5144940	1.9638720
B	-0.0794690	-2.7318820	0.1124580
B	-3.1114590	0.6808340	-0.4160320
B	0.3595630	-2.7028150	1.6866050
B	0.0489700	2.6435050	1.4348380
B	-2.9483590	1.4248730	1.0227460
B	-1.5186790	2.1712900	1.3188440
B	2.9954110	0.4784290	0.9212470
B	2.2445310	-0.0601920	2.3531820
B	0.7136770	0.0887610	2.8644010
B	2.6673230	1.9347220	0.3405370
B	-0.3788140	1.3899830	2.3822700
B	1.1300840	2.6443330	0.2140200
Li	1.0662280	0.4894400	-1.0877060
Li	-1.1395930	0.0518740	0.2074050
F	0.4431960	-0.2245600	0.2059930

^{3}(A@1) Conformer 2.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6787160	-1.7668930	0.9367300
B	0.8581290	-2.4997980	-1.3870040
B	-1.2131730	-2.3789140	1.3597380
B	2.0514370	2.3254040	-0.9840350
B	-0.5193190	2.7620040	-0.0347220
B	-2.8496420	-0.0894460	-1.8776950
B	-0.9440230	-0.0396440	3.1066290
B	2.8345220	-1.0624660	1.4355080
B	-0.2262110	-1.4195690	2.4832380
B	0.1963700	-0.0578160	-3.0342530
B	1.3484750	-1.0384730	-2.4026860
B	2.9533190	0.8777510	-0.7572800
B	0.5458980	2.5978180	-1.5226630
B	-3.0205150	-0.1875850	1.0081950
B	-1.0597100	2.6108740	-1.6079230
B	2.7687770	-0.3730200	-1.7363230
B	-1.7789260	-2.3312780	-0.3308080
B	-0.7662630	-2.8019150	-1.5224340
B	-0.3270640	-1.5153510	-2.4683650
B	-2.8986820	-0.9852640	-0.5293920
B	-1.3833560	-0.0862490	-2.5605510
B	3.0764070	-0.7837080	-0.1634720
B	2.3183250	-1.8818560	-1.3160920
B	-0.4107860	1.3831160	-2.5209490
B	-2.0677150	1.3455480	-1.8556720
B	-2.0519480	0.6839930	2.1362150
B	1.4685750	-1.6399770	2.2244460
B	-0.1527090	-2.8600130	0.0159640
B	-3.0371780	0.7466820	-0.4813170
B	0.3777410	-2.6745390	1.6154570
B	-0.0139370	2.7054250	1.5267230
B	-2.9590890	1.4472930	0.9930540
B	-1.5332980	2.1827930	1.2988590
B	2.9762800	0.5556820	1.0655350
B	2.1155250	-0.0486550	2.4250260
B	0.6387610	0.0883300	3.0250620
B	2.6989600	2.0385450	0.4595210
B	-0.3879380	1.3079860	2.2975990
B	1.1488670	2.6584790	0.4282650
Li	0.9546470	-1.0914380	0.3100570
Li	0.8183870	0.5687300	-1.0378370
F	-0.2194140	0.0425530	0.1197140

^{3}(A@1) Conformer 3.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6780680	-1.8661470	0.9125450
B	0.8707010	-2.5070160	-1.3280300
B	-1.2427920	-2.5008240	1.3536140
B	2.1558910	2.2918540	-1.0809720
B	-0.4252320	3.0171520	-0.0771340
B	-2.7640510	-0.1706010	-1.8771790
B	-0.8773740	-0.0593950	3.0724400
B	2.9311540	-1.0796030	1.4123430
B	-0.2915080	-1.4905200	2.4931600
B	0.2604910	-0.0465510	-3.0591830
B	1.4290540	-0.8914660	-2.3423950
B	2.9907250	0.8320230	-0.8058780
B	0.6143440	2.5503680	-1.4813170
B	-2.8859730	-0.2350060	0.9901610
B	-1.0156040	2.6085480	-1.5858220
B	2.9239330	-0.4726760	-1.7736520
B	-1.8594420	-2.6050810	-0.3054920
B	-0.7211560	-2.7851810	-1.4752950
B	-0.1990110	-1.4859280	-2.3908060
B	-2.8536360	-1.0966230	-0.5355650
B	-1.2916470	-0.1279330	-2.5893610
B	3.1317010	-0.8430450	-0.1542690
B	2.3514320	-1.8645870	-1.2913550
B	-0.3277660	1.3475720	-2.4072670
B	-2.0108250	1.3074410	-1.8245720
B	-1.9267400	0.6874760	2.1025630
B	1.3980070	-1.4292090	2.0274130
B	-0.1434510	-3.0426690	0.0570960
B	-2.9739760	0.6870380	-0.4901060
B	0.3867650	-2.6430660	1.5518180
B	0.0720500	2.7232960	1.4643960
B	-2.8230560	1.4573420	0.9430970
B	-1.4965460	2.3176540	1.4120210
B	3.0022330	0.5103490	0.9675060
B	2.2809340	-0.0514160	2.4514840
B	0.7500410	0.0792880	2.8424250
B	2.7273440	1.9933740	0.3619860
B	-0.3255570	1.3537030	2.3402610
B	1.2108550	2.6980400	0.2980080
Li	-0.7748740	1.0337570	-0.0675300
Li	-0.5142780	-1.0259270	0.0344320
F	0.5846890	0.1393360	-0.0055280

^{2}(B@1)$^{+}$ Conformer 1.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6990190	-1.7705280	0.9350310
B	0.8763000	-2.4910000	-1.4463290
B	-1.1986350	-2.3029740	1.3067300
B	2.1207570	2.3116650	-1.0666490
B	-0.4974720	2.8874100	-0.0147690
B	-2.8279080	-0.1627890	-1.8485120
B	-0.8748590	0.0004820	3.0548660
B	2.9068570	-1.0709280	1.3812250
B	-0.2131170	-1.3928060	2.4833850
B	0.2262380	-0.0053310	-3.0621360
B	1.4032190	-0.9309920	-2.4350480
B	3.0012720	0.8624510	-0.8047430
B	0.5676790	2.5244800	-1.4337140
B	-3.0589360	-0.1840420	1.0501670
B	-1.0773640	2.5701000	-1.5177330
B	2.8582030	-0.4117390	-1.8015360
B	-1.8274140	-2.3761510	-0.3253340
B	-0.7381240	-2.7212250	-1.5050010
B	-0.2402400	-1.4565810	-2.4488080
B	-3.0204650	-1.0752060	-0.5152240
B	-1.3572490	-0.0902690	-2.5824790
B	3.1809310	-0.8403350	-0.2211120
B	2.3664440	-1.8634270	-1.3842450
B	-0.3849940	1.3385860	-2.4125040
B	-2.0771480	1.2979710	-1.7865010
B	-1.9957130	0.7394540	2.1093980
B	1.4867760	-1.5187930	2.1703450
B	-0.1262020	-2.8601340	0.0283030
B	-3.1277230	0.7181080	-0.4954250
B	0.4173310	-2.6011510	1.5521350
B	0.0672600	2.7021390	1.5199130
B	-2.9184070	1.4507860	0.9493580
B	-1.4973770	2.1976210	1.2772710
B	3.0385320	0.5349290	0.9515530
B	2.2515230	-0.0146600	2.3782580
B	0.7321550	0.1125280	2.8735790
B	2.7378840	2.0138020	0.3584310
B	-0.3803770	1.4366040	2.4345270
B	1.1752700	2.6015070	0.3191500
Li	1.1218800	-1.1026640	0.1554020
Li	-1.1592280	-0.0607820	-0.0075380
F	0.4112430	0.3190210	-0.0336270

^{2}(B@1)$^+$ Conformer 2.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.7258990	-1.8162530	0.9105520
B	0.8428040	-2.5427330	-1.3860650
B	-1.2429590	-2.3429620	1.3396840
B	2.0483700	2.3415440	-1.0136580
B	-0.5200690	2.8082620	-0.0325270
B	-2.8248640	-0.1271050	-1.8807490
B	-0.9302270	-0.0272280	3.1358220
B	2.8109260	-1.0985050	1.4384370
B	-0.2790590	-1.4387410	2.5286400
B	0.2119440	-0.0134820	-3.0608070
B	1.3820210	-0.9560290	-2.4588690
B	2.9749890	0.8892450	-0.7423880
B	0.5369320	2.6173400	-1.5350900
B	-2.9689220	-0.2358000	0.9892960
B	-1.0729070	2.6211770	-1.5924000
B	2.7800680	-0.3883530	-1.7375720
B	-1.8287180	-2.4243780	-0.3152350
B	-0.7467610	-2.7655780	-1.4855040
B	-0.2625360	-1.4529530	-2.4085680
B	-2.9239560	-1.0422470	-0.5280800
B	-1.3684440	-0.0793130	-2.5968370
B	3.0624550	-0.8203710	-0.1500420
B	2.2925540	-1.8492770	-1.3229570
B	-0.4232880	1.4097690	-2.5136840
B	-2.0610810	1.3206740	-1.8136640
B	-2.0131730	0.6995230	2.1550980
B	1.4231200	-1.5931740	2.2468360
B	-0.1575020	-2.8975630	0.0640640
B	-3.0403930	0.7130820	-0.5027750
B	0.3542360	-2.6618160	1.6259300
B	0.0241300	2.7034380	1.5127750
B	-2.8896980	1.4281970	0.9545680
B	-1.4983090	2.2106480	1.3226310
B	2.9348370	0.5129140	1.0243590
B	2.1549300	-0.0541410	2.4481910
B	0.6636920	0.0686720	3.0112510
B	2.6396260	2.0075330	0.4306170
B	-0.3602330	1.2925240	2.2950800
B	1.1560250	2.7398730	0.3834750
Li	0.9152920	-1.0991410	0.3047890
Li	0.8046560	0.6010980	-1.0252300
F	-0.2248210	0.0567700	0.1206630

^{2}(B@1)$^+$ Conformer 3.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6496700	-1.8150370	0.9279780
B	0.8790780	-2.5535380	-1.3449960
B	-1.2188260	-2.4693530	1.3516930
B	2.1359700	2.2884960	-1.0589890
B	-0.4649880	2.9684990	-0.0363610
B	-2.7674020	-0.1499500	-1.8897050
B	-0.8733140	-0.0272310	3.0361400
B	2.9233920	-1.0893610	1.4101200
B	-0.2518020	-1.4611370	2.4337920
B	0.2559390	-0.0563730	-3.0207900
B	1.4216060	-0.9521260	-2.3735760
B	2.9919450	0.8400790	-0.7830810
B	0.5997720	2.5457940	-1.4696610
B	-2.9311670	-0.1984760	0.9845670
B	-1.0289070	2.6141770	-1.5734720
B	2.8717060	-0.4607030	-1.7519000
B	-1.8347010	-2.5350940	-0.3032320
B	-0.7204040	-2.8067140	-1.4731560
B	-0.2083350	-1.5069960	-2.3913030
B	-2.8201100	-1.0704130	-0.5321370
B	-1.3094490	-0.1218870	-2.6209510
B	3.1272440	-0.8491080	-0.1707160
B	2.3421390	-1.8804590	-1.2851230
B	-0.3392330	1.3445820	-2.3712470
B	-2.0404630	1.3372820	-1.8500520
B	-1.9483110	0.7552140	2.1291040
B	1.4304500	-1.5112030	2.0377260
B	-0.1365470	-3.0886210	0.0544750
B	-3.0292920	0.7022850	-0.4973740
B	0.4056340	-2.6928450	1.5539530
B	0.0918520	2.7446380	1.4922370
B	-2.8365450	1.4681930	0.9206930
B	-1.4728990	2.3148660	1.3587350
B	3.0033910	0.5261210	0.9857230
B	2.2608140	-0.0687640	2.4096850
B	0.7277250	0.0554960	2.8594650
B	2.7396650	2.0082070	0.3775110
B	-0.3379820	1.3903180	2.3407530
B	1.2136320	2.6938610	0.3143890
Li	-0.8758190	0.9338830	-0.1073680
Li	-0.2659050	-1.0918020	0.0148190
F	0.5898950	0.2403400	0.0516910

^{2}(A@2)$^-$ Conformer 1.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.7066760	-1.7920340	0.9029600
B	0.8809180	-2.4958240	-1.4486520
B	-1.2065320	-2.3114570	1.2849720
B	2.0980200	2.2933190	-1.0192950
B	-0.4986900	2.8318380	-0.0244670
B	-2.8317910	-0.1345270	-1.8798300
B	-0.8827410	-0.0001950	3.0734090
B	2.9112490	-1.0368450	1.4065810
B	-0.2096430	-1.3724980	2.4391260
B	0.2322910	-0.0311770	-3.0321210
B	1.3838090	-0.9851040	-2.3988990
B	2.9603890	0.8531640	-0.7289470
B	0.5661400	2.5245080	-1.4621560
B	-3.0305230	-0.1971620	1.0145180
B	-1.0539570	2.6037060	-1.5710930
B	2.8086360	-0.4055740	-1.7273280
B	-1.7967470	-2.3591980	-0.3613060
B	-0.7507940	-2.7677720	-1.5573290
B	-0.2834110	-1.4879730	-2.4965740
B	-3.0114180	-1.0644450	-0.5503610
B	-1.3550490	-0.0883580	-2.5987800
B	3.2369300	-0.8090260	-0.1924870
B	2.3704460	-1.9102630	-1.3994700
B	-0.3720490	1.3480090	-2.3960350
B	-2.0538740	1.3329720	-1.8227750
B	-1.9922590	0.7176520	2.1196350
B	1.4826910	-1.5304440	2.1496440
B	-0.1362450	-2.8404280	-0.0095540
B	-3.1141040	0.7243100	-0.5077580
B	0.4103240	-2.6014930	1.5431810
B	0.0328380	2.7565710	1.5266780
B	-2.8992660	1.4375440	0.9387990
B	-1.4937320	2.2061890	1.2941200
B	2.9956720	0.6017180	1.0458840
B	2.2399600	-0.0192800	2.4389050
B	0.7171800	0.1167430	2.9372890
B	2.7537540	2.0711240	0.4230630
B	-0.3607030	1.4111660	2.3621920
B	1.1670320	2.6116430	0.3762000
Li	-1.1436890	-0.0662600	-0.1352880
Li	1.1735230	-1.1167180	0.1282130
F	0.4118760	0.2970230	0.0551930

^{2}(A@2)$^-$ Conformer 2.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.7143480	-1.7805700	0.9291180
B	0.9043080	-2.4791700	-1.4203020
B	-1.2191820	-2.3277890	1.3384920
B	2.0734500	2.2861400	-1.0772950
B	-0.5086890	2.8066050	-0.0441420
B	-2.7853400	-0.1468240	-1.8588740
B	-0.9201560	-0.0003460	3.0779570
B	2.8851140	-1.0717380	1.3863540
B	-0.2653590	-1.3945900	2.4904910
B	0.2504540	-0.0031240	-3.0795040
B	1.4296820	-0.8711260	-2.3869980
B	2.9897460	0.8574860	-0.8579190
B	0.5520240	2.5668440	-1.5180110
B	-3.0807440	-0.1887740	1.0423740
B	-1.0580490	2.6211000	-1.5975470
B	2.9774630	-0.4133880	-1.8696880
B	-1.8080230	-2.3867800	-0.3297640
B	-0.7149340	-2.7253480	-1.4900510
B	-0.2016620	-1.4307360	-2.4118240
B	-2.9801860	-1.0588900	-0.5267970
B	-1.3199800	-0.0882980	-2.5921670
B	3.1483340	-0.8382890	-0.2040080
B	2.3814310	-1.8426080	-1.3639110
B	-0.3596300	1.3620850	-2.4219010
B	-2.0328270	1.3247100	-1.7962330
B	-2.0204580	0.7321760	2.1288610
B	1.4589840	-1.5157150	2.2283170
B	-0.1297120	-2.8360160	0.0472890
B	-3.0910980	0.7217030	-0.5014640
B	0.3957500	-2.6085220	1.5958440
B	0.0397110	2.7101870	1.4940220
B	-2.9306210	1.4515930	0.9495050
B	-1.5136650	2.2103240	1.2837050
B	3.0267030	0.5121340	0.9395880
B	2.2115420	-0.0230060	2.3963230
B	0.7029260	0.0953480	2.8866960
B	2.7160630	1.9917460	0.3412320
B	-0.3872010	1.3958630	2.3650800
B	1.1729540	2.6126910	0.3398690
Li	1.1202600	-1.1040760	0.2298430
Li	-1.1458430	-0.0944770	0.1249500
F	0.4005940	0.2866070	-0.1274510

^{2}(A@2)$^-$ Conformer 3.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.7386850	-1.8188610	0.9119850
B	0.8685600	-2.5253170	-1.3755170
B	-1.2633310	-2.3521240	1.3485890
B	2.0595440	2.3436840	-1.0499890
B	-0.5256960	2.8286340	-0.0193680
B	-2.8158550	-0.1113750	-1.8552810
B	-0.9596370	-0.0321630	3.1382710
B	2.7860140	-1.0965040	1.4097060
B	-0.3134070	-1.4379710	2.5286670
B	0.2286450	0.0036620	-3.0423490
B	1.4115930	-0.9398880	-2.4587180
B	3.0155440	0.8991730	-0.8395180
B	0.5401750	2.6236890	-1.5312430
B	-2.9903500	-0.2159740	1.0299540
B	-1.0783300	2.6404380	-1.5897490
B	2.8595460	-0.3696340	-1.8164970
B	-1.8243670	-2.4087040	-0.3170500
B	-0.7364030	-2.7542910	-1.4811370
B	-0.2313030	-1.4527000	-2.4006400
B	-2.9038750	-1.0440320	-0.5259650
B	-1.3469240	-0.0740590	-2.5394290
B	3.0283930	-0.8227210	-0.1707240
B	2.3078740	-1.8408460	-1.3155390
B	-0.4093500	1.4223930	-2.4962330
B	-2.0653060	1.3417230	-1.8172920
B	-2.0401540	0.7080290	2.1656630
B	1.4013750	-1.5785760	2.2763890
B	-0.1658030	-2.8974930	0.0724910
B	-3.0043920	0.7256470	-0.4571880
B	0.3403910	-2.6684930	1.6371920
B	0.0330520	2.6491190	1.5057940
B	-2.9507190	1.4226870	1.0033250
B	-1.5096340	2.1244850	1.2617210
B	2.9498080	0.4950510	0.9904810
B	2.1392210	-0.0609370	2.4419490
B	0.6488940	0.0486590	2.9771810
B	2.6517330	1.9837180	0.3910000
B	-0.3936580	1.3383140	2.3902200
B	1.1480350	2.6846110	0.3446350
Li	0.9044620	-1.0906460	0.3392600
Li	0.8520850	0.5910880	-1.0042500
F	-0.2579820	0.0336480	0.0792620

^{2}(A@2)$^-$ Conformer 4.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6828530	-1.8196070	0.8920100
B	0.8524110	-2.5970610	-1.4555140
B	-1.1853270	-2.3437020	1.2903210
B	2.1083560	2.2395740	-1.0556660
B	-0.5087690	2.8275710	-0.0409070
B	-2.8356630	-0.1606160	-1.9017630
B	-0.8835600	-0.0501570	3.0462480
B	2.9834280	-1.1674390	1.4282240
B	-0.2106530	-1.4516670	2.4374140
B	0.2050170	-0.0819920	-3.0839930
B	1.3752610	-0.9585090	-2.3928460
B	3.0394010	0.8002280	-0.7262120
B	0.5908910	2.4520210	-1.4748570
B	-2.9690300	-0.2226370	1.0040400
B	-1.0589420	2.5437000	-1.5657520
B	2.8163950	-0.4620830	-1.7287920
B	-1.8085490	-2.4354560	-0.3620400
B	-0.7361200	-2.8385150	-1.5319690
B	-0.2611980	-1.5060030	-2.4141390
B	-2.9142800	-1.0599020	-0.5376180
B	-1.3814200	-0.1407340	-2.6511370
B	3.1408290	-0.9275900	-0.1677520
B	2.2946820	-1.9023630	-1.3069580
B	-0.3749630	1.2936020	-2.4183340
B	-2.0623210	1.2922530	-1.8434600
B	-2.0114590	0.7355440	2.1580680
B	1.4619280	-1.5556920	2.0311110
B	-0.1014330	-2.8394740	0.0091450
B	-3.1292340	0.7076860	-0.5252000
B	0.4038130	-2.6913320	1.5614500
B	0.1022800	2.6433880	1.4750050
B	-2.9100680	1.4341610	0.9480590
B	-1.5007890	2.2138380	1.3294410
B	3.1214090	0.5169230	1.0281000
B	2.2603800	-0.0836840	2.3804990
B	0.7333220	0.0521510	2.8605870
B	2.7391400	1.9610820	0.4131960
B	-0.3653750	1.3695920	2.3911350
B	1.2130410	2.7345180	0.2744170
Li	-1.1107630	0.6420990	-0.0200120
Li	1.1246620	0.5690550	0.5395980
F	0.0859070	-0.4176300	-0.1530860

^{2}(A@2)$^-$ Conformer 5.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6573360	-1.8047550	0.9491610
B	0.8939970	-2.4933020	-1.4404640
B	-1.1787740	-2.3730780	1.3251160
B	2.1358380	2.3267110	-1.0362870
B	-0.4642110	2.7777400	-0.0230490
B	-2.7666390	-0.1751260	-1.8724600
B	-0.8838050	-0.0066420	3.1147130
B	2.9055280	-1.0078330	1.3986730
B	-0.1912410	-1.4350520	2.5525830
B	0.2439310	-0.1033340	-3.1340870
B	1.4192970	-1.0513000	-2.4808620
B	2.9846070	0.8746470	-0.7704890
B	0.6031260	2.4838170	-1.4799360
B	-2.9908300	-0.2050830	1.0530720
B	-0.9971650	2.5351340	-1.5808840
B	2.7899970	-0.3804130	-1.7554840
B	-1.7565270	-2.3775130	-0.3329080
B	-0.7405160	-2.7440600	-1.5760510
B	-0.2767360	-1.6164220	-2.6995720
B	-2.8807390	-1.0567180	-0.5072980
B	-1.3495140	-0.1405880	-2.6895450
B	3.1546840	-0.7624410	-0.1962320
B	2.3169810	-1.8354020	-1.2988210
B	-0.3379750	1.3046230	-2.4842110
B	-1.9738530	1.2618670	-1.8338950
B	-2.0341010	0.7913610	2.2448600
B	1.4451120	-1.4402490	2.0601920
B	-0.0864730	-2.7970970	-0.0107080
B	-2.9684250	0.6904380	-0.4778020
B	0.4281910	-2.6030030	1.5646010
B	0.0680540	2.7220100	1.5334110
B	-2.8847980	1.4326150	0.9786620
B	-1.4728600	2.1959200	1.3159540
B	2.9799630	0.6090010	1.0012560
B	2.2716120	0.0056230	2.4390680
B	0.7344100	0.1141220	2.9193720
B	2.7950610	2.1004740	0.3883980
B	-0.3829930	1.4491260	2.4717110
B	1.1988840	2.5991440	0.3713910
Li	-0.1040360	-0.5715170	-0.9863130
Li	-0.8656510	-0.2442050	0.9148110
F	0.5257120	0.2659010	0.2104100

^{2}(A@2)$^-$ Conformer 6.

PBE1PBE/6-31+g(d)

Atom	X	Y	Z
B	-2.6893710	-1.8702160	0.9332130
B	0.8905770	-2.4902630	-1.3471260
B	-1.2253310	-2.4896480	1.3718520
B	2.0830400	2.2493850	-1.0871250
B	-0.5682460	3.0853870	-0.0483270
B	-2.7447720	-0.1850110	-1.8666390
B	-0.8430890	-0.0299210	3.0395750
B	2.9893390	-1.1347490	1.4555510
B	-0.2143150	-1.4471940	2.4542180
B	0.2826390	-0.0119220	-3.0333660
B	1.4254180	-0.9128060	-2.3259970
B	3.0726500	0.8319330	-0.7436440
B	0.5888320	2.5651170	-1.5036800
B	-2.9406450	-0.2456880	1.0212340
B	-1.0816450	2.6711240	-1.5778620
B	2.9064500	-0.4600410	-1.7299240
B	-1.8473670	-2.5641580	-0.3185200
B	-0.7151570	-2.7537100	-1.4860570
B	-0.1842680	-1.4684990	-2.4202460
B	-2.8885980	-1.1100320	-0.5273910
B	-1.2853190	-0.0914770	-2.5691520
B	3.1131100	-0.9028310	-0.1417500
B	2.3920010	-1.9022640	-1.3218230
B	-0.3518190	1.4077630	-2.4428970
B	-1.9969700	1.3074600	-1.8020910
B	-1.9485900	0.7323760	2.1298100
B	1.4571280	-1.5275420	2.0139240
B	-0.1346360	-2.9579120	0.0460320
B	-2.9647000	0.6681450	-0.4829210
B	0.4010750	-2.6941420	1.5727710
B	0.0605690	2.7138310	1.4377880
B	-2.8793220	1.4088890	0.9597910
B	-1.4983550	2.2179160	1.2943060
B	2.9975710	0.5032440	0.9718260
B	2.2837840	-0.0817990	2.4052750
B	0.7511320	0.0527950	2.8512580
B	2.6663150	1.9601520	0.3762420
B	-0.3472310	1.4074430	2.3604400
B	1.1665310	2.7282460	0.2293840
Li	-0.3879390	1.0951160	-0.2235700
Li	-0.7804200	-0.8583760	0.1581480
F	0.6397280	-0.1009770	0.0575270

^{3}(A@1)

UPBE1PBE/6-311+g(2d)

Atom	X	Y	Z
B	2.5151140	0.8293140	1.9766960
B	-0.7275360	2.9113990	0.0795340
B	0.9836220	1.1628340	2.4750560
B	-1.9238480	-1.2317960	-2.2761010
B	0.5295410	-2.3682340	-1.5029730
B	3.0504290	0.9635180	-1.2213850
B	0.5002250	-1.6983990	2.6060500
B	-3.0821020	0.2776950	1.4365270
B	-0.1298960	-0.1838380	2.7735390
B	0.1483080	1.6922630	-2.4916800
B	-1.0744930	2.2004930	-1.5498160
B	-2.8480160	-0.1342550	-1.3677370
B	-0.3490550	-1.2578620	-2.6331700
B	2.8760040	-0.5562830	1.2273410
B	1.2585900	-1.3698310	-2.6128780
B	-2.5836550	1.4340510	-1.4981050
B	1.7904900	2.0281420	1.1255510
B	0.9040680	3.1293430	0.3033710
B	0.6086030	2.5887970	-1.2205170
B	3.0314500	0.9858590	0.4006380
B	1.6815840	1.4111990	-1.9936850
B	-3.1857920	0.9752220	-0.0497440
B	-2.2002830	2.4781370	-0.3538470
B	0.6786150	0.1712340	-2.6875940
B	2.2867470	-0.2387430	-2.0622200
B	1.7368210	-1.8345130	1.5431950
B	-1.7721380	0.2356620	2.4829260
B	0.0884830	2.3656900	1.5153110
B	3.1826070	-0.5119780	-0.5226090
B	-0.6242370	1.3655060	2.6648350
B	-0.1619480	-3.1558310	-0.2536580
B	2.7802910	-1.8833320	0.2704310
B	1.3551110	-2.6529030	0.0048940
B	-3.1210190	-0.8868450	0.2401970
B	-2.5065300	-1.1559710	1.7987370
B	-1.0667430	-1.6446070	2.3106760
B	-2.7653770	-1.7770860	-1.0513090
B	0.0732390	-2.4245200	1.1829950
B	-1.1757050	-2.2995310	-1.1667420
Li	-1.1916700	0.9038170	0.6032790
Li	1.1511690	0.0416580	-0.0650170
F	-0.4171360	-0.2906710	-0.1276230

^{2}(B@1)$^{+}$

UPBE1PBE/6-311+g(2d)

Atom	X	Y	Z
B	2.7255880	1.5064790	1.2224150
B	-0.8394390	2.7344840	-0.9358010
B	1.2458890	1.9875540	1.7063530
B	-2.1608930	-2.0211760	-1.4630440
B	0.4436330	-2.8324790	-0.5717660
B	2.8102090	0.4623600	-1.8071600
B	0.8911950	-0.5964000	2.9763810
B	-2.8728670	0.8321910	1.5852670
B	0.2537960	0.8876800	2.6951130
B	-0.2456720	0.5919660	-2.9904200
B	-1.3978520	1.3973900	-2.1912530
B	-3.0160130	-0.6405640	-0.9254930
B	-0.6222980	-2.1880930	-1.8846760
B	3.0604160	-0.0716870	1.0319950
B	1.0175380	-2.2413120	-1.9845320
B	-2.8537840	0.7955320	-1.6540230
B	1.8632530	2.3599660	0.1158200
B	0.7741800	2.9378790	-0.9611670
B	0.2521970	1.8882720	-2.1215480
B	3.0254510	1.1001390	-0.3320980
B	1.3393540	0.5581200	-2.5273280
B	-3.1607330	0.9224830	-0.0246310
B	-2.3350150	2.1302620	-0.9817200
B	0.3431680	-0.8569600	-2.6251760
B	2.0400260	-0.9662010	-2.0240400
B	1.9923110	-1.1625720	1.9049470
B	-1.4436770	1.1023560	2.4305530
B	0.1782980	2.7950270	0.5733220
B	3.1051800	-0.6640630	-0.6558930
B	-0.3574850	2.2591750	2.0214310
B	-0.1068180	-2.9308130	0.9710590
B	2.8881280	-1.6489890	0.6216520
B	1.4626320	-2.4217710	0.8154700
B	-3.0328380	-0.6538510	0.8595100
B	-2.2260910	-0.3986350	2.3508140
B	-0.7140520	-0.6484830	2.7993930
B	-2.7626530	-1.9894710	-0.0081470
B	0.3686710	-1.8779300	2.1047610
B	-1.2184520	-2.5893870	-0.1730480
Li	-1.0994380	1.0742150	0.3786240
Li	1.1557170	0.0246180	-0.0144970
F	-0.4243430	-0.2961610	-0.0886820

^{2}(A@2)$^{-}$

UPBE1PBE/6-311+g(2d)

Atom	X	Y	Z
B	2.6733540	0.8946220	1.8156770
B	-0.6821570	2.9382030	-0.0141290
B	1.1738980	1.2512890	2.3365270
B	-2.0768950	-1.3016180	-2.1456020
B	0.4037160	-2.4455060	-1.4430010
B	2.9646480	0.8745950	-1.4019730
B	0.6354490	-1.6100910	2.6655460
B	-2.9723160	0.3770450	1.5826070
B	0.0583180	-0.0687340	2.7912580
B	0.0074130	1.5790550	-2.5910340
B	-1.1553380	2.1543600	-1.6244350
B	-2.9140440	-0.1572590	-1.2123540
B	-0.5323100	-1.3813780	-2.5756610
B	2.9353250	-0.5484700	1.1159280
B	1.0831810	-1.5029280	-2.6197800
B	-2.6419630	1.4144050	-1.4127350
B	1.8899140	2.0855320	0.9799330
B	0.9575650	3.1101990	0.1126300
B	0.5278240	2.5221190	-1.3674850
B	3.0685220	0.9875770	0.2177840
B	1.5550580	1.3025390	-2.1182020
B	-3.1763860	1.0160550	0.0822830
B	-2.1809960	2.5095850	-0.3488720
B	0.5121050	0.0361100	-2.7234110
B	2.1421590	-0.3572200	-2.1454670
B	1.7916100	-1.8228990	1.5447970
B	-1.5971520	0.3369800	2.5468010
B	0.2293830	2.4358270	1.4454650
B	3.1125070	-0.5746890	-0.6526560
B	-0.4431170	1.4810370	2.6258090
B	-0.2427800	-3.1308850	-0.1050430
B	2.7567510	-1.9001890	0.2105940
B	1.3107930	-2.6493860	0.0538620
B	-3.0802090	-0.8392670	0.4367820
B	-2.4088250	-1.0574440	1.9794960
B	-0.9466200	-1.5425990	2.4169500
B	-2.8358940	-1.7947260	-0.8328870
B	0.1257800	-2.4279740	1.3140920
B	-1.2775150	-2.3509310	-1.0712840
Li	-1.1373080	0.9700550	0.6192690
Li	1.1464640	0.0465320	-0.0426330
F	-0.4276420	-0.2589050	-0.1250470

^{1}(B@2)

UPBE1PBE/6-311+g(2d)

Atom	X	Y	Z
B	2.6742830	1.7882260	0.8830330
B	-0.9037320	2.4966420	-1.4700140
B	1.1818530	2.3329630	1.2625110
B	-2.0569620	-2.3111410	-1.0029970
B	0.5230380	-2.8198790	0.0091200
B	2.7808730	0.1280430	-1.8595110
B	0.8923380	0.0500840	3.0414280
B	-2.8924770	1.0821120	1.3852980
B	0.2059350	1.4183470	2.4188630
B	-0.2485270	-0.0357470	-3.0500560
B	-1.4180090	0.8764590	-2.4313330
B	-2.9747200	-0.8926660	-0.7551440
B	-0.5450170	-2.5722000	-1.4633800
B	3.0586350	0.2164820	1.0295240
B	1.0604300	-2.6234840	-1.5413600
B	-2.8495520	0.3668530	-1.7716970
B	1.7876480	2.3760980	-0.3749290
B	0.6977220	2.7124440	-1.5493690
B	0.2115550	1.4091510	-2.4601060
B	2.9705850	1.0612650	-0.5531120
B	1.3218270	0.0547990	-2.5889700
B	-3.1658930	0.8214700	-0.2065480
B	-2.3732480	1.8319430	-1.4022920
B	0.3610880	-1.3931020	-2.3854440
B	2.0364130	-1.3386850	-1.7737750
B	2.0190960	-0.6913670	2.1348150
B	-1.4915280	1.5920940	2.1491820
B	0.1080150	2.8605770	-0.0160750
B	3.1094220	-0.7195430	-0.5007770
B	-0.4250540	2.6444670	1.5250010
B	-0.0199270	-2.7099570	1.5435770
B	2.9104890	-1.4116620	0.9567570
B	1.5124090	-2.1872630	1.3236410
B	-2.9826870	-0.5299140	0.9858620
B	-2.2029810	0.0673650	2.3957400
B	-0.6999750	-0.0864320	2.9183120
B	-2.6843370	-2.0161650	0.4165550
B	0.3773120	-1.3706890	2.3711970
B	-1.1533320	-2.6454970	0.4009770
Li	-1.1157830	1.1203250	0.1579320
Li	1.1584650	0.0138640	0.0390840
F	-0.4138180	-0.2964040	-0.0531340

FLi_2. Neutral doublet.

UPBE1PBE/6-311+g(2d)

Atom	X	Y	Z
Li	0.0000000	1.3211750	-0.6212150
Li	0.0000000	-1.3211750	-0.6212150
F	0.0000000	0.0000000	0.4141430

FLi_2. Positively charged singlet.

UPBE1PBE/6-311+g(2d)

Atom	X	Y	Z
Li	0.0000000	1.6671150	-0.0520900
Li	0.0000000	-1.6671150	-0.0525560
F	0.0000000	0.0000000	0.0348820

References:

S1. 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, 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, Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Wallingford CT2009.

S2. E. D. Glendening, K. B. J, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis and F. Weinhold., Theoretical Chemistry Institute, University of Wisconsin, Madison, 6.0. edn., 2013.

S3. Neese, F. The Orca Program System. Wiley Interdiscip. Rev.: Comput. Mol. Sci. 2012, 2, 73-78.

S4. M. Lundberg and P. E. M. Siegbahn, *J. Chem. Phys.*, 2005, **122**, 224103.

S5. M. Sodupe, J. Bertran, L. Rodríguez-Santiago and E. J. Baerends, *J. Phys. Chem. A* 1999, **103**, 166-170.

S6. J. Gräfenstein, E. Kraka and D. Cremer *Phys. Chem. Chem. Phys.* 2004, **6**, 1096-1112.

S7. J. Poater, M. Solà, A. Rimola, L. Rodríguez-Santiago and M. Sodupe, *J. Phys. Chem. A* 2004, **108**, 6072-6078.

S8. Zhurko G. A. Chemcraft - graphical program for visualization of quantum chemistry computations. (https://chemcraftprog.com)