Electronic Structure and Thermochemical Properties of Small Neutral and Cationic Lithium Clusters and Boron-Doped Lithium Clusters: $Li_n^{0/+}$ and $Li_nB^{0/+}$ (n = 1 - 8)

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Supporting Information: Energies and equilibrium geometries calculated at the B3LYP/aug-cc-pVTZ level. Energy contributions and equilibrium geometries calculated at the CCSD(T) level. Kohn-Sham orbitals for the closed shell clusters.

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Table S1. Energy contributions calculated at the CCSD(T) level for Li_n and Li_n^+ (n = 1 – 8).

Molecule	ZPE [a]	$H_{298K} - H_{0K}$ [a]	VDZ	VTZ	VQZ	CBS	CV [b]	SR [c]	T_1
Li (^{2}S)	0.000000	0.002360	-7.432420	-7.432679	-7.432695	-7.432697	-0.038872	-0.000674	0.004
Li^+ (^{1}S)	0.000000	0.002360	-7.236119	-7.236380	-7.236384	-7.236378	-0.037258	-0.000661	0.000
Li_2 ($^1\Sigma_g^+$)	0.000794	0.003668	-14.900635	-14.903184	-14.903693	-14.903949	-0.077987	-0.001349	0.012
Li_2^+ ($^2\Sigma_g^+$)	0.000595	0.003776	-14.715109	-14.715971	-14.716193	-14.716313	-0.076586	-0.001335	0.002
Li_3 ($^2B_2$)	0.001543	0.005366	-22.352666	-22.356958	-22.357849	-22.358302	-0.117247	-0.002020	0.015
Li_3^+ ($^1A_1'$)	0.001742	0.005221	-22.203751	-22.207192	-22.208119	-22.208626	-0.116147	-0.002013	0.008
Li_4 (^1A_g) [d]	0.003093	0.007010	-29.831171	-29.837507	-29.838803	-29.839459	-0.156668	-0.002694	0.013
Li_4^+ ($^2B_{1u}$) [d]	0.002520	0.007366	-29.661734	-29.666470	-29.667627	-29.668245	-0.155497	-0.002685	0.008
Li_5 ($^2B_2$)	0.004708	0.008487	-37.29329	-37.303049	-37.30486	-37.305745	-0.196415	-0.003365	0.013
Li_5^+ ($^1A_1'$)	0.004587	0.008561	-37.146917	-37.15504	-37.156832	-37.305745	-0.195332	-0.003355	0.010
Li_6 ($^1A_{1g}$)	0.005979	0.010507	-44.774280	-44.787290	-44.789013	-44.789726	-0.235806	-0.004036	0.013
Li_6^+ ($^2A_1$)	0.005716	0.010559	-44.619560	-44.629595	-44.631202	-44.631940	-0.234490	-0.004027	0.032
Li_7 ($^2A_2''$)	0.007356	0.012068	-52.253553	-52.267660	-52.269583	-52.270392	-0.275151	-0.004711	0.009
Li_7^+ ($^1A_1'$)	0.007269	0.012061	-52.109296	-52.121788	-52.123778	-52.124690	-0.274238	-0.004702	0.013
Li_8 ($^1A_1$)	0.008545	0.013951	-59.730211	-59.745912	-59.748087	-59.749011	-0.315719	-0.005393	0.015
Li_8^+ ($^2A'$)	0.008654	0.014109	-59.574939	-59.589667	-59.591703	-59.592568	-0.313948	-0.005377	0.024

[a] CCSD(T)/VQZ for n = 1 – 5, and CCSD(T)/VTZ for n = 6 – 8. [b] CCSD(T)/cc-pwCVTZ.

[c] E[CCSD(T)-DK/cc-pwCVTZ-DK] – E[CCSD(T)/cc-pwCVTZ].

[d] ZPE and thermal correction (H_{298K} - H_{0K}) calculated at the B3LYP/aug-cc-pVDZ level are 0.003037 and 0.007010 a.u. for Li_4, and 0.002520 and 0.007366 a.u. for Li_4^+.

Table S2. Energy contributions calculated at the CCSD(T) level for Li_n and Li_n^+ (n = 1 – 8).

Molecule	ZPE [a]	$H_{298K} - H_{0K}$ [a]	aVDZ	aVTZ	aVQZ	CBS	CV [b]	SR [c]	T_1
B (^{2}P)	0.000000	0.002360	-24.591078	-24.598424	-24.600921	-24.602355	-0.043699	-0.006734	0.010
LiB ($^3\Pi$)	0.001231	0.003499	-32.0626772	-32.0750506	-32.0783846	-32.080210	-0.083342	-0.007352	0.019
LiB ($^1\Sigma^+$)	0.000955	0.003596	-32.052721	-32.065258	-32.068806	-32.070770	-0.082971	-0.007386	0.019
LiB ($^3\Sigma^+$)	0.001395	0.003458	-32.044681	-32.057686	-32.061166	-32.063068	-0.083531	-0.007351	0.010
LiB^+ ($^2\Sigma$)	0.000757	0.003678	-31.8548709	-31.8641999	-31.8668214	-31.868286	-0.081706	-0.007399	0.016
LiB^+ ($^2\Pi$)	0.000497	0.003837	-31.830500	-31.839326	-31.841967	-31.843447	-0.081429	-0.007386	0.008
Li_2B ($^4A_2$)	0.002934	0.004769	-39.5490535	-39.5658092	-39.5700358	-39.572312	-0.123324	-0.008001	0.014
Li_2B ($^2\Pi_u$)	0.003008	0.005076	-39.540935	-39.558945	-39.563648	-39.566202	-0.123054	-0.008005	0.012
Li_2B^+ ($^1\Sigma_g^+$)	0.003147	0.004902	-39.383141	-39.400073	-39.404451	-39.406824	-0.121673	-0.008023	0.007
Li_2B^+ ($^3\Pi_g$)	0.002379	0.004496	-39.373650	-39.388730	-39.392314	-39.394214	-0.121451	-0.008012	0.006
Li_3B ($^1A_1$)	0.004533	0.006286	-47.032115	-47.053070	-47.058391	-47.061262	-0.162684	-0.008680	0.026
Li_3B^+ ($^4A_2$")	0.004304	0.006547	-46.883528	-46.903168	-46.907607	-46.909926	-0.161618	-0.008648	0.005
Li_3B^+ ($^2B_2$)	0.004459	0.006339	-46.876454	-46.897074	-46.902217	-46.904979	-0.161568	-0.008395	0.008
Li_4B ($^2B_2$, C_{2v})	0.006504	0.007651	-54.532506	-54.557715	-54.563775	-54.566997	-0.203152	-0.009336	0.041
Li_4B ($^2B_2$, D_{2d})	0.006604	0.007812	-54.531498	-54.557043	-54.563373	-54.566767	-0.203269	-0.009321	0.011
Li_4B ($^2A_{2u}$, D_{4h})	0.006581	0.006887	-54.530484	-54.556369	-54.562716	-54.566109	-0.203300	-0.009322	0.012
Li_4B^+ ($^1A_{1g}$)	0.006701	0.007551	-54.379759	-54.405235	-54.411545	-54.414928	-0.201911	-0.009316	0.007
Li_5B ($^1A_1$)	0.008971	0.008796	-62.043519	-62.072756	-62.079746	-62.083458	-0.243548	-0.009997	0.033

Li_5B^+ ($^2A_1$)	0.008372	0.009217	-61.883761	-61.913084	-61.920072	-61.923778	-0.242531	-0.009971	0.008
Li_6B ($^2A_{1g}$)	0.010880	0.010235	-69.546497	-69.579661	-69.587186	-69.591122	-0.283755	-0.010668	0.013
Li_6B^+ ($^1A_{1g}$)	0.011088	0.010040	-69.405913	-69.438473	-69.446152	-69.450214	-0.283058	-0.010637	0.007
Li_7B ($^1A_1'$)	0.011872	0.012094	-77.023546	-77.058186	-77.065876	-77.069872	-0.323168	-0.011351	0.016
Li_7B^+ ($^2A_1'$)	0.011765	0.012075	-76.867046	-76.901035	-76.908797	-76.912864	-0.322345	-0.011325	0.011
Li_8B ($^2A'$)	0.013241	0.013616	-84.478622	-84.514946	-84.522906	-84.527026	-0.363068	-0.012015	0.030
Li_8B^+ ($^1A_1$)	0.013094	0.013716	-84.338733	-84.375326	-84.383450	-84.387672	-0.362735	-0.012021	0.013

[a] CCSD(T)/aVQZ for n = 1 – 5, and CCSD(T)/aVTZ for n = 6 – 8. [b] CCSD(T)/aug-cc-pwCVTZ.

[c] E[CCSD(T)-DK/aug-cc-pwCVTZ-DK] – E[CCSD(T)/aug-cc-pwCVTZ].

Table S3. Molecular and electronic symmetry and energy at 0 K for the lowest isomers of Li_n and Li_n^+ (n = 1 – 8) at the G3B3 level.

Molecule	Label	Symm	State	E_{0K}	Molecule	Label	Symm	State	E_{0K}
Li_2	**2.1**	$D_{\infty h}$	$^1\Sigma^+_g$	-14.972341	Li_6	**6.4**	D_{5h}	$^1A_1'$	-44.985209
Li_2^+	**2c.1**	$D_{\infty h}$	$^2\Sigma^+_g$	-14.780686		**6.5**	D_{3h}	$^1A_1'$	-44.983281
Li_3	**3.1**	C_{2v}	$^2B_2$	-22.459672	Li_6^+	**6c.1**	C_{2v}	$^2A_1$	-44.831565
Li_3^+	**3c.1**	D_{3h}	$^1A_1'$	-22.306647		**6c.2**	D_{2h}	$^2B_{2u}$	-44.831235
Li_4	**4.1**	D_{2h}	^1A_g	-29.975565		**6c.3**	O_h	$^4A_{1g}$	-44.813287
Li_4^+	**4c.1**	D_{2h}	$^2B_{1u}$	-29.800500	Li_7	**7.1**	D_{5h}	$^2A_2''$	-52.509344
	4c.2	C_{2v}	$^2A_1$	-29.797609		**7.2**	C_{3v}	$^2A_1$	-52.500419
Li_5	**5.1**	C_{2v}	$^2B_2$	-37.474732	Li_7^+	**7c.1**	D_{5h}	$^1A_1'$	-52.359705
	5.2	C_{2v}	$^2A_1$	-37.470980		**7c.2**	C_{3v}	$^1A_1$	-52.350795
	5.3	D_{3h}	$^4A_2''$	-37.464903	Li_8	**8.1**	T_d	$^1A_1$	-60.023201
Li_5^+	**5c.1**	D_{3h}	$^1A_1'$	-37.323592		**8.2**	C_{3v}	$^1A_1$	-60.023909
	5c.2	D_{2d}	$^1A_1$	-37.316379		**8.4**	C_s	^1A	-60.022739
	5c.3	D_{2h}	^1A_g	-37.315405		**8.3**	C_{2v}	$^1A_1$	-60.023805
Li_6	**6.1**	D_{4h}	$^1A_{1G}$	-44.995337	Li_8^+	**8c.1**	C_s	^2A	-59.858210
	6.3	C_{5v}	$^1A_1$	-44.986566		**8c.2**	C_{2v}	$^2B_1$	-59.851871

Table S4. Electronic state and energy at 0 K for the lowest isomers of Li_nB and Li_n^+B (n = 1 – 8) at the G3B3 level.

Molecule	**Label**	**State**	**E_{0K}**	**Molecule**	**Label**	**State**	**E_{0K}**
LiB	**B1**	$^3\Pi$	-32.155928	LiB^+	**B1c**	$^2\sum$	-31.941105
Li_2B	**B2.1**	$^4A_2$	-39.681026	Li_2B^+	**B2c.1**	$^1\sum_g^+$	-39.510859
Li_3B	**B3.1**	$^1A_1$	-47.20371	Li_3B^+	**B3c.1**	$^4A_2$"	-47.049057
Li_4B	**B4.1**	$^2B_2$	-54.74459	Li_4B^+	**B4c.1**	$^1A_{1g}$	-54.585535
Li_5B	**B5.1**	$^1A_1$	-62.294781	Li_5B^+	**B5c.1**	$^2A_1$	-62.129571
Li_6B	**B6.1**	$^2A_{1g}$	-69.831342	Li_6B^+	**B6c.1**	$^1A_{1G}$	-69.689736
Li_7B	**B7.1**	$^1A_1$'	-77.348568	Li_7B^+	**B7c.1**	$^2A_1$'	-77.185784
Li_8B	**B8.1**	^2A’	-84.839618	Li_8B^+	**B8c.1**	$^1A_1$	-84.697861
				Li_8B^+	**B8c.2**	$^1A_1$	-84.701061

Table S5. Equilibrium geometries calculated at the CCSD(T) level for Li_n and Li_n^+ (n = 1 – 8).

	Basis set	Coordinate			
Li_2 ($^1\Sigma^+_g$)	cc-pVQZ	3	0.000000000	0.000000000	1.349228230
		3	0.000000000	0.000000000	-1.349228230
Li_2^+ ($^2\Sigma^+_g$)	cc-pVQZ	3	0.000000000	0.000000000	1.565922801
		3	0.000000000	0.000000000	-1.565922801
Li_3 ($^2B_2$)	cc-pVQZ	3	0.000000000	1.635993921	-0.752866398
		3	0.000000000	0.000000000	1.505732796
		3	0.000000000	-1.635993921	-0.752866398
Li_3^+ ($^1A_1'$)	cc-pVQZ	3	0.049079328	1.731226733	0.000000000
		3	-1.523825995	-0.823109422	0.000000000
		3	1.474746667	-0.908117311	0.000000000
Li_4 (^1A_g)	cc-pVQZ	3	-2.707406584	0.000000000	0.000000000
		3	0.000000000	-1.331700016	0.000000000
		3	0.000000000	1.331700016	0.000000000
		3	2.707406584	0.000000000	0.000000000
Li_4^+ ($^2B_{1u}$)	cc-pVQZ	LI	0.00000000	0.00000000	-2.84650113
		LI	0.00000000	0.00000000	2.84650113
		LI	0.00000000	1.37922989	0.00000000
		LI	0.00000000	-1.37922989	0.00000000
Li_5 ($^2B_2$)	cc-pVQZ	3	0.000000000	2.571784111	-0.005122808
		3	0.000000000	-2.571784111	-0.005122808
		3	0.000000000	0.000000000	1.505691845
		3	-1.525437360	0.000000000	-0.747723115
		3	1.525437360	0.000000000	-0.747723115
Li_5^+ ($^1A_1'$)	cc-pVQZ	3	0.000000000	1.597032714	0.000000000
		3	-1.383070901	-0.798516357	0.000000000
		3	1.383070901	-0.798516357	0.000000000
		3	0.000000000	0.000000000	2.741249521
		3	0.000000000	0.000000000	-2.741249521
Li_6 ($^1A_{1g}$)	cc-pVTZ	LI	0.00000000	0.00000000	1.38326005
		LI	0.00000000	0.00000000	-1.38326005

		LI	0.00000000	2.55008479	0.00000000
		LI	0.00000000	-2.55008479	0.00000000
		LI	2.55008479	0.00000000	0.00000000
		LI	-2.55008479	0.00000000	0.00000000
Li_6^+ ($^2A_1$)	cc-pVTZ	LI	-1.33790587	0.00000000	-0.42768300
		LI	1.33790587	0.00000000	-0.42768300
		LI	0.00000000	1.73704405	1.71203019
		LI	0.00000000	-1.73704405	1.71203019
		LI	0.00000000	2.72271227	-1.28434720
		LI	0.00000000	-2.72271227	-1.28434720
Li_7 ($^2A_2$")	cc-pVTZ	LI	0.00000000	2.65001505	0.00000000
		LI	0.00000000	0.00021328	1.47578116
		LI	0.00000000	0.00021328	-1.47578116
		LI	-1.55812650	-2.14447425	0.00000000
		LI	1.55812650	-2.14447425	0.00000000
		LI	-2.52039942	0.81925344	0.00000000
		LI	2.52039942	0.81925344	0.00000000
Li_7^+ ($^1A_1$')	cc-pVTZ	LI	0.00000000	2.78878652	0.00000000
		LI	0.00000000	0.00000000	1.30735345
		LI	0.00000000	0.00000000	-1.30735345
		LI	-1.63921589	-2.25617360	0.00000000
		LI	1.63921589	-2.25617360	0.00000000
		LI	-2.65230307	0.86178034	0.00000000
		LI	2.65230307	0.86178034	0.00000000
Li_8 ($^1A_1$)	cc-pVTZ	LI	0.00000000	0.00000000	1.74739518
		LI	0.00000000	0.00000000	-3.05769171
		LI	-2.49659483	-1.44140970	1.01923057
		LI	2.49659483	-1.44140970	1.01923057
		LI	0.00000000	2.88281940	1.01923057
		LI	0.00000000	-1.64745997	-0.58246506
		LI	1.42674219	0.82372998	-0.58246506
		LI	-1.42674219	0.82372998	-0.58246506

Li_8^+ ($^2A'$)	cc-pVTZ	LI	0.12553666	-1.13518370	2.62726481
		LI	0.12553666	-1.13518370	-2.62726481
		LI	-0.96737580	1.59767507	-1.60020604
		LI	-0.96737580	1.59767507	1.60020604
		LI	1.42576847	2.92207042	0.00000000
		LI	0.91599501	-2.87919867	0.00000000
		LI	-1.56851924	-1.10253543	0.00000000
		LI	0.91045808	0.13474155	0.00000000

Table S6. Equilibrium geometries in Angstroms calculated at the CCSD(T) level for Li_nB and Li_n^+B (n = 1 – 8).

	Basis set	**Coordinate**			
LiB ($^3\Pi$)	aVQZ	B	0.00000000	0.00000000	-0.83931614
		LI	0.00000000	0.00000000	1.30716143
LiB ($^1\Sigma^+$)	aVQZ	B	0.00000000	0.00000000	-0.93875788
		LI	0.00000000	0.00000000	1.46203323
LiB ($^3\Sigma^+$)	aVQZ	B	0.00000000	0.00000000	-0.77313447
		LI	0.00000000	0.00000000	1.20408928
LiB^+ ($^2\Sigma^+$)	aVQZ	B	0.00000000	0.00000000	-0.97043015
		LI	0.00000000	0.00000000	1.51136003
LiB^+ ($^2\Pi$)	aVQZ	B	0.00000000	0.00000000	-1.00189406
		LI	0.00000000	0.00000000	1.56036231
Li_2B ($^4A_2$)	aVQZ	LI	0.00000000	1.60777740	-0.60504029
		LI	0.00000000	-1.60777740	-0.60504029
		B	0.00000000	0.00000000	0.71948750
Li_2B ($^2\Pi_u$)	aVQZ	B	0.00000000	0.00000000	0.00000000
		LI	0.00000000	0.00000000	2.18601613
		LI	0.00000000	0.00000000	-2.18601613
Li_2B^+ ($^1\Sigma_g^+$)	aVQZ	LI	0.00000000	0.00000000	2.30136669
		LI	0.00000000	0.00000000	-2.30136669
		B	0.00000000	0.00000000	0.00000000
Li_2B^+ ($^3\Pi_g$)	aVQZ	B	0.00000000	0.00000000	0.00000000
		LI	0.00000000	0.00000000	2.23977636
		LI	0.00000000	0.00000000	-2.23977636
Li_3B ($^1A_1$)	aVQZ	LI	0.00000000	2.18703089	0.42648404
		LI	0.00000000	-2.18703089	0.42648404
		B	0.00000000	0.00000000	0.56739934
		LI	0.00000000	0.00000000	-1.73005046
Li_3B^+ ($^4A_2$")	aVQZ	B	0.00000000	0.00000000	0.00000000
		LI	2.13631193	0.00000000	0.00000000

		LI	-1.06815597	-1.85010040	0.00000000
		LI	-1.06815597	1.85010040	0.00000000
Li_3B^+ ($^2B_2$)	aVQZ	B	0.00000000	0.00000000	0.21562199
		LI	0.00000000	0.00000000	2.43343058
		LI	0.00000000	1.57128756	-1.38462147
		LI	0.00000000	-1.57128756	-1.38462147
Li_4B ($^2B_2$, C_{2v})	aVQZ	LI	0.00000000	1.35147055	-1.09157634
		LI	0.00000000	-1.35147055	-1.09157634
		LI	-2.15399707	0.00000000	0.57517547
		LI	2.15399707	0.00000000	0.57517547
		B	0.00000000	0.00000000	0.64393069
Li_4B ($^2B_2$, D_{2d})	aVQZ	B	0.00000000	0.00000000	0.00000000
		LI	0.00000000	-2.05695966	0.54145787
		LI	0.00000000	2.05695966	0.54145787
		LI	2.05695966	0.00000000	-0.54145787
		LI	-2.05695966	0.00000000	-0.54145787
Li_4B ($^2A_{2u}$, D_{4h})	aVQZ	B	0.00000000	0.00000000	0.00000000
		LI	2.14585998	0.00000000	0.00000000
		LI	-2.14585998	0.00000000	0.00000000
		LI	0.00000000	-2.14585998	0.00000000
		LI	0.00000000	2.14585998	0.00000000
Li_4B^+ ($^1A_{1g}$)	aVQZ	LI	0.00000000	2.22743586	0.00000000
		LI	0.00000000	-2.22743586	0.00000000
		LI	2.22743586	0.00000000	0.00000000
		LI	-2.22743586	0.00000000	0.00000000
		B	0.00000000	0.00000000	0.00000000
Li_5B ($^1A_1$)	aVQZ	3	2.136227617	0.000000000	-0.272716222
		3	0.000000000	2.136227617	-0.272716222
		3	0.000000000	0.000000000	1.772232431
		3	0.000000000	-2.136227617	-0.272716222
		3	-2.136227617	0.000000000	-0.272716222
		5	0.000000000	0.000000000	-0.445564004

Li_5B^+ ($^2A_1$)	aVQZ	3	2.179958023	0.000000000	-0.385715388
		3	0.000000000	-2.179958023	-0.385715388
		3	0.000000000	2.179958023	-0.385715388
		3	0.000000000	0.000000000	1.873391415
		3	-2.179958023	0.000000000	-0.385715388
		5	0.000000000	0.000000000	-0.202935273
Li_6B ($^2A_{1g}$)	aVQZ	3	0.000000000	0.000000000	2.152956688
		3	0.000000000	2.152956688	0.000000000
		3	2.152956688	0.000000000	0.000000000
		3	-2.152956688	0.000000000	0.000000000
		3	0.000000000	0.000000000	-2.152956688
		3	0.000000000	-2.152956688	0.000000000
		5	0.000000000	0.000000000	0.000000000
Li_6B^+ ($^1A_{1g}$)	aVQZ	3	0.000000000	0.000000000	2.165990128
		3	0.000000000	2.165990128	0.000000000
		3	0.000000000	0.000000000	-2.165990128
		3	2.165990128	0.000000000	0.000000000
		3	0.000000000	-2.165990128	0.000000000
		3	-2.165990128	0.000000000	0.000000000
		5	0.000000000	0.000000000	0.000000000
Li_7B ($^1A_1'$)	aVTZ	LI	0.00000000	-2.28664625	0.00000000
		LI	0.00000000	0.00001346	-2.17039959
		LI	0.00000000	0.00001346	2.17039959
		LI	-2.17472437	-0.70661665	0.00000000
		LI	2.17472437	-0.70661665	0.00000000
		LI	1.34404973	1.84992841	0.00000000
		LI	-1.34404973	1.84992841	0.00000000
		B	0.00000000	-0.00000413	0.00000000
Li_7B^+ ($^2A_1'$)	aVTZ	LI	2.18916951	0.71130429	0.00000000
		LI	-2.18916951	0.71130429	0.00000000
		LI	0.00000000	0.00000000	-2.19464945
		LI	0.00000000	0.00000000	2.19464945

		LI	1.35298116	-1.86221881	0.00000000
		LI	-1.35298116	-1.86221881	0.00000000
		LI	0.00000000	2.30182903	0.00000000
		B	0.00000000	0.00000000	0.00000000
Li_8B ($^2A'$)	aVTZ	B	-0.01713297	0.11440197	0.00000000
		LI	0.99860497	-1.64971025	1.36358083
		LI	0.99860497	-1.64971025	-1.36358083
		LI	-0.80751242	2.29828241	0.00000000
		LI	-1.31099683	0.24858001	-1.85760148
		LI	-1.31099683	0.24858001	1.85760148
		LI	-1.30824899	-1.99652486	0.00000000
		LI	1.38352676	1.15897736	1.43788279
		LI	1.38352676	1.15897736	-1.43788279

Table S7. Equilibrium geometries in Angstroms calculated at the B3LYP/aug-cc-pVTZ level.

Structures	Label	ES	Cartesian Coordinates			
Li_2	**2.1**	$^1\Sigma^+_g$	3	0.000000000	0.000000000	1.349526000
			3	0.000000000	0.000000000	-1.349526000
Li_2^+	**2c.1**	$^2\Sigma^+_g$	3	0.000000000	0.000000000	1.535658000
			3	0.000000000	0.000000000	-1.535658000
Li_3	**3.1**	$^2B_2$	3	0.000000000	1.315702000	-0.916603000
			3	0.000000000	0.000000000	1.833206000
			3	0.000000000	-1.315702000	-0.916603000
Li_3^+	**3c.1**	$^1A_1'$	3	0.000000000	1.702988000	0.000000000
			3	1.474831000	-0.851494000	0.000000000
			3	-1.474831000	-0.851494000	0.000000000
Li_4	**4.1**	^1A_g	3	0.000000000	0.000000000	2.718004000
			3	0.000000000	1.286767000	0.000000000
			3	0.000000000	-1.286767000	0.000000000
			3	0.000000000	0.000000000	-2.718004000
Li_4^+	**4c.1**	$^2B_{1u}$	3	0.000000000	0.000000000	2.788679000
			3	0.000000000	1.351505000	0.000000000
			3	0.000000000	-1.351505000	0.000000000
			3	0.000000000	0.000000000	-2.788679000
	4c.2	$^2A_1$	3	0.000000000	0.000000000	0.553950000
			3	0.000000000	1.429272000	-2.098381000
			3	0.000000000	-1.429272000	-2.098381000
			3	0.000000000	0.000000000	3.642811000
Li_5	**5.1**	$^2B_2$	3	0.000000000	1.510451000	-0.712251000
			3	0.000000000	-1.510451000	-0.712251000
			3	0.000000000	0.000000000	1.440097000
			3	-2.556636000	0.000000000	-0.007797000
			3	2.556636000	0.000000000	-0.007797000
	5.2	$^2A_1$	3	0.000000000	1.528115000	-1.527067000
			3	0.000000000	0.000000000	0.913859000
			3	0.000000000	-1.528115000	-1.527067000
			3	0.000000000	-2.985827000	1.070138000
			3	0.000000000	2.985827000	1.070138000
	5.3	$^4A_2''$	3	0.000000000	1.712222000	0.000000000
			3	-1.482828000	-0.856111000	0.000000000
			3	1.482828000	-0.856111000	0.000000000
			3	0.000000000	0.000000000	2.296865000
			3	0.000000000	0.000000000	-2.296865000
Li_5^+	**5c.1**	$^1A_1'$	3	0.000000000	1.550923000	0.000000000
			3	-1.343139000	-0.775462000	0.000000000
			3	1.343139000	-0.775462000	0.000000000
			3	0.000000000	0.000000000	2.735030000
			3	0.000000000	0.000000000	-2.735030000
	5c.1	$^1A_1$	3	0.000000000	1.407899000	2.720410000

			3	0.000000000	0.000000000	0.000000000
			3	-1.407899000	0.000000000	-2.720410000
			3	1.407899000	0.000000000	-2.720410000
			3	0.000000000	-1.407899000	2.720410000
	5c.3	$^{1}A_{g}$	3	0.000000000	2.750632000	1.408929000
			3	0.000000000	0.000000000	0.000019000
			3	0.000000000	-2.750632000	1.408929000
			3	0.000000000	-2.750717000	-1.408939000
			3	0.000000000	2.750717000	-1.408939000
Li_6	**6.1**	$^{1}A_{1G}$	3	1.263231000	0.000000000	-0.000023000
			3	-1.263231000	0.000000000	-0.000023000
			3	0.000000000	1.762702000	-1.762698000
			3	0.000000000	-1.762702000	-1.762698000
			3	0.000000000	1.762631000	1.762721000
			3	0.000000000	-1.762631000	1.762721000
	6.2	$^{3}B_{1}$	3	-1.421679000	0.000000000	-0.391832000
			3	1.421679000	0.000000000	-0.391832000
			3	0.000000000	1.513792000	1.567436000
			3	0.000000000	-1.513792000	1.567436000
			3	0.000000000	2.493653000	-1.175604000
			3	0.000000000	-2.493653000	-1.175604000
	6.3	$^{1}A_{1}$	3	0.000000000	2.678275000	-0.129660000
			3	0.000000000	0.000000000	0.648301000
			3	-1.574251000	-2.166770000	-0.129660000
			3	1.574251000	-2.166770000	-0.129660000
			3	-2.547191000	0.827632000	-0.129660000
			3	2.547191000	0.827632000	-0.129660000
	6.4	$^{1}A_{1}'$	3	0.000000000	2.742681000	0.000000000
			3	0.000000000	0.000000000	0.000000000
			3	1.612107000	-2.218875000	0.000000000
			3	-1.612107000	-2.218875000	0.000000000
			3	2.608444000	0.847535000	0.000000000
			3	-2.608444000	0.847535000	0.000000000
	6.5	$^{1}A_{1}'$	3	0.000000000	1.718131000	0.000000000
			3	1.487945000	-0.859066000	0.000000000
			3	-1.487945000	-0.859066000	0.000000000
			3	-2.969050000	1.714182000	0.000000000
			3	2.969050000	1.714182000	0.000000000
			3	0.000000000	-3.428363000	0.000000000
Li_6^+	**6c.1**	$^{2}A_{1}$	3	-1.259305000	0.000000000	-0.390102000
			3	1.259305000	0.000000000	-0.390102000
			3	0.000000000	1.680170000	1.655126000
			3	0.000000000	-1.680170000	1.655126000
			3	0.000000000	2.638933000	-1.265025000
			3	0.000000000	-2.638933000	-1.265025000
	6c.2	$^{2}B_{2u}$	3	0.000000000	0.000000000	1.253171000

			3	0.000000000	0.000000000	-1.253171000
			3	-2.185634000	1.537286000	0.000000000
			3	2.185634000	1.537286000	0.000000000
			3	-2.185634000	-1.537286000	0.000000000
			3	2.185634000	-1.537286000	0.000000000
	6c.3	$^4A_{1g}$	3	-2.133618000	0.000000000	-0.000006000
			3	2.133618000	0.000000000	-0.000006000
			3	0.000000000	1.501753000	1.501760000
			3	0.000000000	-1.501753000	1.501760000
			3	0.000000000	1.501775000	-1.501754000
			3	0.000000000	-1.501775000	-1.501754000
	6c.4	$^2B_2$	3	0.000000000	0.000000000	2.915212000
			3	0.000000000	0.000000000	-0.044830000
			3	0.000000000	1.521712000	-2.449407000
			3	0.000000000	-1.521712000	-2.449407000
			3	0.000000000	2.535721000	1.014216000
			3	0.000000000	-2.535721000	1.014216000
	6c.5	$^4A_2$"	3	0.000000000	2.719567000	0.000000000
			3	0.000000000	0.000000000	0.000000000
			3	1.598521000	-2.200176000	0.000000000
			3	-1.598521000	-2.200176000	0.000000000
			3	2.586462000	0.840392000	0.000000000
			3	-2.586462000	0.840392000	0.000000000
Li_7	**7.1**	$^2A_2$"	3	0.000000000	2.569200000	0.000000000
			3	0.000000000	0.000000000	1.357513000
			3	-1.510138000	-2.078527000	0.000000000
			3	1.510138000	-2.078527000	0.000000000
			3	-2.443454000	0.793926000	0.000000000
			3	2.443454000	0.793926000	0.000000000
			3	0.000000000	0.000000000	-1.357513000
	7.2	$^2A_1$	3	0.000000000	-1.710782000	-1.032351000
			3	0.000000000	2.897744000	0.633040000
			3	2.509520000	-1.448872000	0.633040000
			3	0.000000000	0.000000000	1.197933000
			3	-1.481580000	0.855391000	-1.032351000
			3	1.481580000	0.855391000	-1.032351000
			3	-2.509520000	-1.448872000	0.633040000
Li_7^+	**7c.1**	$^1A_1$'	3	0.000000000	2.704293000	0.000000000
			3	0.000000000	0.000000000	1.212243000
			3	-1.589544000	-2.187819000	0.000000000
			3	1.589544000	-2.187819000	0.000000000
			3	-2.571936000	0.835673000	0.000000000
			3	2.571936000	0.835673000	0.000000000
			3	0.000000000	0.000000000	-1.212243000
	7c.2	$^1A_1$	3	0.000000000	-1.880352000	-0.832543000
			3	0.000000000	3.161805000	0.448057000

			3	2.738204000	-1.580903000	0.448057000
			3	0.000000000	0.000000000	1.153459000
			3	-1.628432000	0.940176000	-0.832543000
			3	1.628432000	0.940176000	-0.832543000
			3	-2.738204000	-1.580903000	0.448057000
Li_8	**8.1**	$^1A_1$	3	1.008859000	1.008859000	1.008859000
			3	-1.765359000	-1.765359000	-1.765359000
			3	-1.765359000	1.765359000	1.765359000
			3	1.765359000	1.765359000	-1.765359000
			3	-1.008859000	-1.008859000	1.008859000
			3	1.008859000	-1.008859000	-1.008859000
			3	-1.008859000	1.008859000	-1.008859000
			3	1.765359000	-1.765359000	1.765359000
	8.2	$^1A_1$	3	0.000000000	0.000000000	0.172443000
			3	1.593689000	0.920117000	-1.620137000
			3	0.000000000	2.537975000	0.640613000
			3	2.197951000	-1.268987000	0.640613000
			3	-1.593689000	0.920117000	-1.620137000
			3	0.000000000	-1.840233000	-1.620137000
			3	-2.197951000	-1.268987000	0.640613000
			3	0.000000000	0.000000000	2.766132000
	8.4	$^1A'$	3	1.104871000	2.458870000	-0.047350000
			3	-1.563759000	-1.455837000	0.972764000
			3	-2.691372000	-0.000001000	-1.658262000
			3	2.696947000	0.000277000	-1.107703000
			3	-1.563973000	1.455436000	0.972960000
			3	0.949464000	-0.000006000	1.728929000
			3	-0.037546000	-0.000014000	-0.813819000
			3	1.105368000	-2.458726000	-0.047519000
	8.3	$^1A_1$	3	0.000000000	0.000000000	-0.179162000
			3	0.000000000	0.000000000	2.410700000
			3	1.796981000	1.631349000	0.519276000
			3	-1.796981000	1.631349000	0.519276000
			3	1.796981000	-1.631349000	0.519276000
			3	-1.796981000	-1.631349000	0.519276000
			3	0.000000000	-1.640328000	-2.154321000
			3	0.000000000	1.640328000	-2.154321000
Li_8^+	**8c.1**	$^2A'$	3	1.150034000	2.609577000	-0.115114000
			3	-1.575338000	-1.514457000	0.959667000
			3	-2.935453000	0.000009000	-1.437780000
			3	2.801887000	0.000060000	-0.919958000
			3	-1.575376000	1.514369000	0.959723000
			3	1.043900000	-0.000009000	1.527243000
			3	-0.059786000	-0.000002000	-0.858635000
			3	1.150131000	-2.609547000	-0.115146000
	8c.2	$^2B_1$	3	0.000000000	0.000000000	-1.444954000

			3	0.000000000	0.000000000	2.855912000
			3	1.418178000	1.498251000	0.543865000
			3	-1.418178000	1.498251000	0.543865000
			3	1.418178000	-1.498251000	0.543865000
			3	-1.418178000	-1.498251000	0.543865000
			3	0.000000000	-2.948823000	-1.793208000
			3	0.000000000	2.948823000	-1.793208000

Table S8. Equilibrium geometries in Angstroms calculated at the B3LYP/aug-cc-pVTZ level

Structures	Label	ES	Coordinates			
LiB	**B1**	$^3\Pi$	LI	0.000000	0.000000	-1.331537
			B	0.000000	0.000000	0.798922
		$^1\Sigma^+$	LI	0.000000	0.000000	-1.495112
			B	0.000000	0.000000	0.897067
		$^3\Sigma^+$	LI	0.000000	0.000000	-1.220436
			B	0.000000	0.000000	0.732262
LiB^+	**B1c**	$^2\Sigma^+$	LI	0.000000	0.000000	-1.537886
			B	0.000000	0.000000	0.922732
		$^2\Pi$	LI	0.000000	0.000000	-1.547011
			B	0.000000	0.000000	0.928207
Li_2B	**B2.1**	$^4A_2$	LI	0.000000	1.557440	-0.613242
			B	0.000000	0.000000	0.735891
			LI	0.000000	-1.557440	-0.613242
	B2.2	$^2\Pi_u$	LI	0.000000	0.000000	2.172818
			B	0.000000	0.000000	0.000000
			LI	0.000000	0.000000	-2.172818
	B2.3	$^2B_2$	LI	0.000000	1.413487	-0.811554
			B	0.000000	0.000000	0.973865
			LI	0.000000	-1.413487	-0.811554
Li_2B^+	**B2c.1**	$^1\sum_g^+$	LI	0.000000	0.000000	2.290888
			B	0.000000	0.000000	0.000000
			LI	0.000000	0.000000	-2.290888
	B2c.2	$^3\Pi_g$	LI	0.000000	0.000000	2.215840
			B	0.000000	0.000000	0.000000
			LI	0.000000	0.000000	-2.215840
Li_3B	**B3.1**	$^1A_1$	LI	0.000000	2.142106	0.507759
			B	0.000000	0.000000	0.458355
			LI	0.000000	-2.142106	0.507759
			LI	0.000000	0.000000	-1.779443
	B3.2	$^1A_1$'	LI	0.000000	2.129631	0.000000
			B	0.000000	0.000000	0.000000
			LI	1.844315	-1.064816	0.000000
			LI	-1.844315	-1.064816	0.000000
Li_3B^+	**B3c.1**	$^4A_2$"	LI	0.000000	2.110997	0.000000
			B	0.000000	0.000000	0.000000
			LI	1.828177	-1.055498	0.000000
			LI	-1.828177	-1.055498	0.000000
	B3c.2	$^2B_2$	LI	0.000000	1.544270	-1.379099
			B	0.000000	0.000000	0.208537
			LI	0.000000	-1.544270	-1.379099
			LI	0.000000	0.000000	2.410637
Li_4B	**B4.1**	$^2B_2$	3	0.000000000	2.055381000	0.421118000
			3	0.000000000	-2.055381000	0.421118000

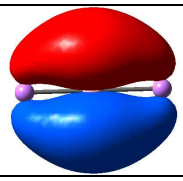
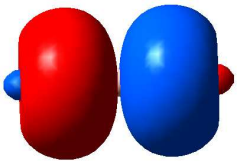
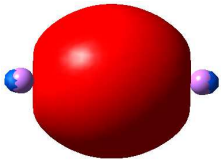
			3	2.055381000	0.000000000	-0.421118000
			3	-2.055381000	0.000000000	-0.421118000
			5	0.000000000	0.000000000	0.000000000
	B4.2	$^2B_2$	3	0.000000000	1.342036000	-1.080215000
			3	0.000000000	-1.342036000	-1.080215000
			3	-2.118178000	0.000000000	0.594127000
			3	2.118178000	0.000000000	0.594127000
			5	0.000000000	0.000000000	0.583305000
	B4.3	$^2A_{2u}$	3	0.000000000	2.111283000	0.000000000
			3	2.111283000	0.000000000	0.000000000
			3	-2.111283000	0.000000000	0.000000000
			3	0.000000000	-2.111283000	0.000000000
			5	0.000000000	0.000000000	0.000000000
Li_4B^+	**B4c.1**	$^1A_{1g}$	3	0.000000000	2.197118000	0.000000000
			3	2.197118000	0.000000000	0.000000000
			3	-2.197118000	0.000000000	0.000000000
			3	0.000000000	-2.197118000	0.000000000
			5	0.000000000	0.000000000	0.000000000
	B4c.2	$^1A_1$	3	0.000000000	1.326333000	-1.510689000
			3	0.000000000	-1.326333000	-1.510689000
			3	-1.834388000	0.000000000	1.347141000
			3	1.834388000	0.000000000	1.347141000
			5	0.000000000	0.000000000	0.196257000
Li_5B	**B5.1**	$^1A_1$	3	-1.481831000	-1.476549000	-0.300822000
			3	1.476567000	-1.481791000	-0.300915000
			3	0.000133000	-0.000007000	1.792530000
			3	-1.476602000	1.481770000	-0.300816000
			3	1.481768000	1.476583000	-0.300912000
			5	-0.000021000	-0.000004000	-0.353439000
	B5.2	$^1A_1$'	3	0.000000000	2.070906000	0.000000000
			3	-1.793457000	-1.035453000	0.000000000
			3	0.000000000	0.000000000	2.087928000
			3	0.000000000	0.000000000	-2.087928000
			5	0.000000000	0.000000000	0.000000000
			3	1.793457000	-1.035453000	0.000000000
	B5.3	$^1A_1$	3	0.000000000	1.658524000	-1.193611000
			3	0.000000000	-1.658524000	-1.193611000
			3	-2.094067000	0.000000000	0.071235000
			3	2.094067000	0.000000000	0.071235000
			5	0.000000000	0.000000000	0.067119000
			3	0.000000000	0.000000000	2.132888000
Li_5B^+	**B5c.1**	$^2A_1$	3	-1.513462000	-1.515474000	-0.378410000
			3	-1.515221000	1.513719000	-0.378403000
			3	1.515730000	-1.513617000	-0.377473000
			3	-0.001308000	-0.000012000	1.835463000
			3	1.513970000	1.515381000	-0.377464000

			5	0.000175000	0.000002000	-0.194228000
Li_6B	**B6.1**	$^2A_{1g}$	3	-1.532148000	0.698000000	1.275712000
			3	1.387171000	1.258058000	0.977335000
			3	0.436887000	-1.546628000	1.370718000
			3	-0.436887000	1.546628000	-1.370718000
			3	1.532148000	-0.698000000	-1.275712000
			3	-1.387171000	-1.258058000	-0.977335000
			5	0.000000000	0.000000000	0.000000000
Li_6B^+	**B6c.1**	$^1A_{1g}$	3	-0.099529000	1.411591000	1.583718000
			3	0.863920000	1.475172000	-1.260300000
			3	1.937765000	-0.585178000	0.643227000
			3	-1.937764000	0.585178000	-0.643228000
			3	0.099528000	-1.411591000	-1.583717000
			3	-0.863920000	-1.475173000	1.260299000
			5	0.000000000	0.000000000	0.000000000
Li_7B	**B7.1**	$^1A_1$'	3	-0.214997000	-2.220716000	0.001067000
			3	0.000307000	-0.001407000	-2.123408000
			3	-2.178674000	-0.481973000	-0.000072000
			3	0.000886000	0.001003000	2.123503000
			3	2.045905000	-0.890228000	0.000330000
			3	1.478578000	1.670717000	-0.001340000
			3	-1.131973000	1.922724000	-0.000130000
			5	-0.000019000	-0.000072000	0.000030000
	B7.2	$^1A_1$	3	1.814354000	-0.113518000	0.000000000
			3	-0.213164000	1.160174000	1.382806000
			3	-0.213164000	1.160174000	-1.382806000
			3	-0.213164000	-1.948776000	-1.483997000
			3	-0.213164000	-1.948776000	1.483997000
			3	1.891249000	3.010004000	0.000000000
			3	-2.388914000	-0.580503000	0.000000000
			5	-0.278421000	-0.443266000	0.000000000
Li_7B^+	**B7c.1**	$^2A_1$'	3	-2.182452000	0.585313000	-0.000455000
			3	0.000120000	-0.000510000	2.159407000
			3	-1.230901000	-1.894509000	0.000356000
			3	0.000414000	-0.000719000	-2.159310000
			3	-0.117784000	2.256484000	-0.000013000
			3	2.109363000	0.809414000	0.000180000
			3	1.421516000	-1.755945000	-0.000212000
			5	-0.000166000	0.000283000	0.000028000
	B7c.2	$^2A_1$	3	1.822597000	-0.256700000	0.000000000
			3	-0.215435000	1.141377000	1.427985000
			3	-0.215435000	1.141377000	-1.427985000
			3	-0.215435000	-1.898981000	-1.552102000
			3	-0.215435000	-1.898981000	1.552102000
			3	1.995036000	2.909131000	0.000000000
			3	-2.433274000	-0.376883000	0.000000000

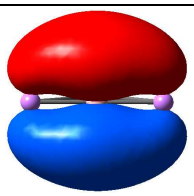
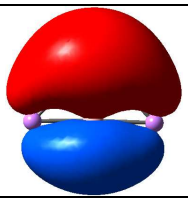
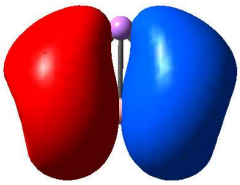
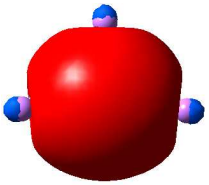
			5	-0.313573000	-0.456204000	0.000000000
Li_8B	**B8.1**	$^2A'$	5	-0.102118000	0.000073000	0.014187000
			3	1.610468000	1.331523000	-0.977962000
			3	-2.239796000	-0.000995000	0.787198000
			3	1.610205000	-1.331339000	-0.978582000
			3	-0.245477000	-1.816778000	1.285293000
			3	1.946353000	-0.000378000	1.276912000
			3	-1.132697000	1.408482000	-1.350725000
			3	-1.133146000	-1.406151000	-1.352595000
			3	-0.245713000	1.815514000	1.286815000
	B8.2	$^2A_{2u}$	3	0.000000000	1.632134000	1.365950000
			3	-1.413469000	-0.816067000	1.365950000
			3	1.413469000	-0.816067000	1.365950000
			3	1.413469000	0.816067000	-1.365950000
			3	-1.413469000	0.816067000	-1.365950000
			3	0.000000000	0.000000000	4.029271000
			3	0.000000000	-1.632134000	-1.365950000
			5	0.000000000	0.000000000	0.000000000
			3	0.000000000	0.000000000	-4.029271000
	B8.3	$^2B_{2g}$	5	0.000000000	0.000000000	0.000000000
			3	0.000000000	1.881564000	1.281454000
			3	-1.881564000	0.000000000	-1.281454000
			3	1.881564000	0.000000000	-1.281454000
			3	0.000000000	-1.881564000	-1.281454000
			3	1.881564000	0.000000000	1.281454000
			3	-1.881564000	0.000000000	1.281454000
			3	0.000000000	1.881564000	-1.281454000
			3	0.000000000	-1.881564000	1.281454000
	B8.4	$^2B_2$	5	0.000000000	0.000000000	0.029425000
			3	0.000000000	1.989779000	1.159142000
			3	-1.377254000	-1.377254000	-1.171403000
			3	1.377254000	1.377254000	-1.171403000
			3	1.377254000	-1.377254000	-1.171403000
			3	1.989779000	0.000000000	1.159142000
			3	-1.989779000	0.000000000	1.159142000
			3	-1.377254000	1.377254000	-1.171403000
			3	0.000000000	-1.989779000	1.159142000
Li_8B^+	**B8c.1**	$^1A_1$	5	0.000000000	0.000000000	0.000000000
			3	0.000000000	1.958082000	1.221480000
			3	-1.384573000	-1.384573000	-1.221480000
			3	1.384573000	1.384573000	-1.221480000
			3	1.384573000	-1.384573000	-1.221480000
			3	1.958082000	0.000000000	1.221480000
			3	-1.958082000	0.000000000	1.221480000
			3	-1.384573000	1.384573000	-1.221480000
			3	0.000000000	-1.958082000	1.221480000

	B8c.2	$^1A_1$	3	0.000000000	1.706776000	-1.301752000
			3	1.478111000	-0.853388000	-1.301752000
			3	-1.478111000	-0.853388000	-1.301752000
			3	-1.470258000	0.848854000	1.318015000
			3	1.470258000	0.848854000	1.318015000
			3	0.000000000	0.000000000	-4.268244000
			3	0.000000000	-1.697708000	1.318015000
			5	0.000000000	0.000000000	0.002714000
			3	0.000000000	0.000000000	4.214932000

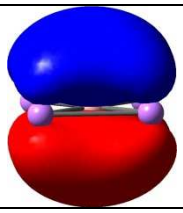
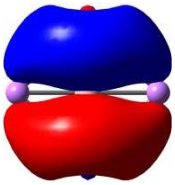
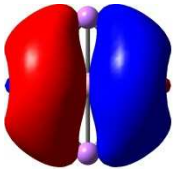
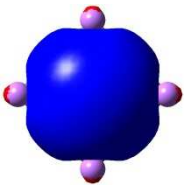
Figure S1. MO diagrams of global minima for closed shell Li_nB using the B3LYP/6-311+G(d) densities.

			
LUMO	HOMO	HOMO-1	

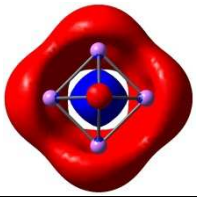
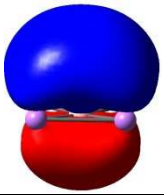
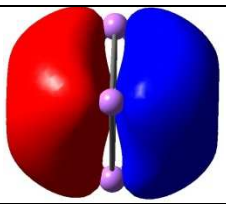
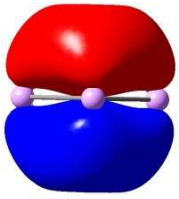
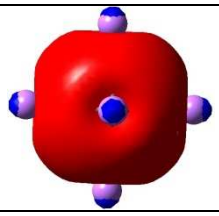
a) Li_2B^+ ($^1\Sigma_g^+$)

			
LUMO	HOMO	HOMO-1	HOMO-2

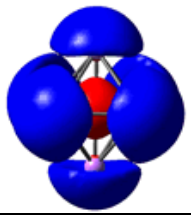
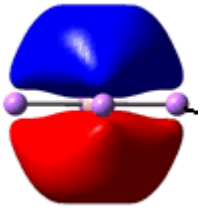
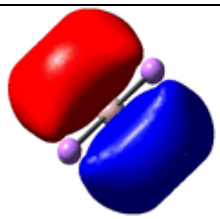
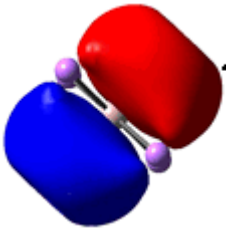
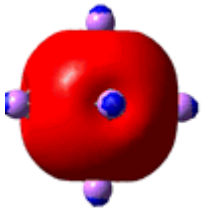
b) Li_3B ($^1A_1$)

			
LUMO	HOMO	HOMO’	HOMO-1

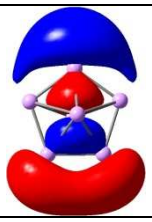
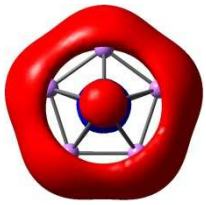
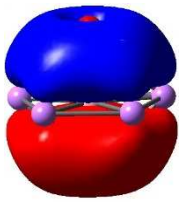
c) Li_4B^+ (D_{4h}, ^1A_g)

		
LUMO	HOMO	HOMO-1
		
HOMO-1’	HOMO-2	

d) Li_5B (C_{4v}, $^1A_1$)

		
LIMO	HOMO	HOMO-1
		
HOMO-1’	HOMO-2	

e) Li_6B^+ ($^1A_{1g}$)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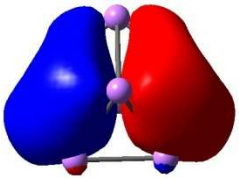
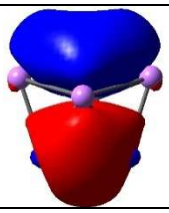
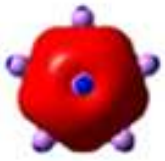
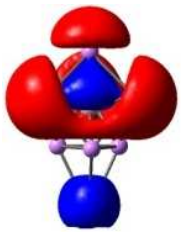
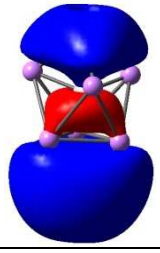
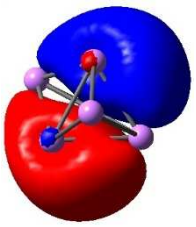
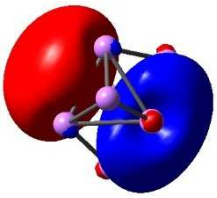
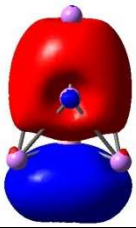
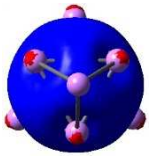
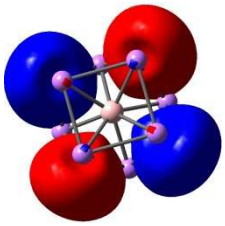
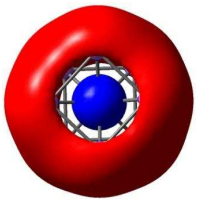
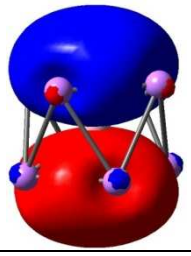
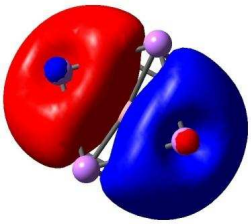
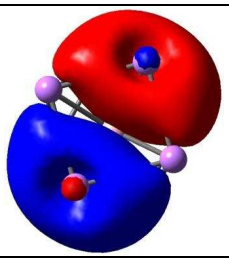
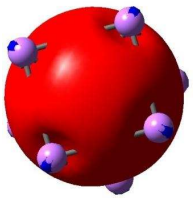
		
HOMO-2	HOMO-2’	HOMO-3

f) Li_7B (D_{5h}, $^1A_1'$)

		
LUMO	HOMO	HOMO-1
		
HOMO-1’	HOMO-2	HOMO-3

g) MOs pictures of Li_8B^+ (C_{3v}, $^1A_1$)

		
LUMO	HOMO	HOMO-1
		
HOMO-2	HOMO-2’	HOMO-3

h) MOs pictures of Li_8B^+ (D_{4d}, $^1A_1$)