

TABLE S1: Natural Charges in Electrons for B_2Li_n ($n = 1-4$) Clusters.

Isomer	Atom	Charge	Isomer	Atom	Charge
1a	B	-0.37	3e	B	-0.71
	Li	0.73		Li(1)	0.38
1b	B	-0.43		Li(4)	0.52
	Li	0.85	4a	B	-1.18
2a	B	-0.73		Li	0.59
	Li	0.73	4b	B(1)	-1.02
2b	B	-0.86		B(2)	-1.55
	Li	0.86		Li(3)	0.63
2c	B	-0.67		Li(6)	0.67
	Li	0.67	4c	B	-1.26
3a	B	-1.16		Li(3)	0.57
	Li	0.77		Li(5)	0.69
3b	B(1)	-0.44	4d	B	-1.31
	B(2)	-1.38		Li(3)	0.63
	Li(3)	0.55		Li(5)	0.68
	Li(5)	0.71	4e	B(1)	-0.76
3c	B(1)	-0.78		B(2)	-0.66
	B(2)	-1.14		Li(3)	0.74
	Li(3)	0.64		Li(4)	0.52
	Li(5)	0.65		Li(5)	0.57
3d	B	-0.94		Li(6)	-0.40
	Li(3)	0.53			
	Li(4)	0.68			
3d'	B	-0.96			
	Li(3)	0.53			
	Li(4)	0.70			

TABLE S2: Frequencies (in cm^{-1}) for the Global Minimum Structures of B_2Li_n ($n=1-4$).

Compound	Frequencies
B_2Li (1a , ${}^2\text{B}_1$)	316(b_2), 512(a_1), 1118(a_1)
B_2Li_2 (2a , ${}^1\text{A}_1$)	133(a_1), 331(b_1), 405(a_2), 517(a_1), 574(b_2), 1168(a_1)
B_2Li_3 (3a , ${}^2\text{A}_1'$)	96(e'), 217(a_2''), 368(e''), 482(a_1'), 580(e'), 1133(a_1')
B_2Li_4 (4a , ${}^1\text{A}_{1g}$)	129(b_{2u}), 224(e_u), 241(a_{2u}), 267(b_{2g}), 322(e_g), 434(b_{1g}), 460(a_{1g}), 548(e_u), 1184(a_{1g})