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Structures and Electronic Properties of Exohedral Metalloborospherenes $Al_{12}Li_{20}\&B_{60}$ and $Al_{20}Li_{12}\&B_{60}$ and Their Endohedral Systems: Push Electron Oxidation of Super-reduced Polyanionic States B_{60}^{50-} and B_{60}^{60-}

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Table S1. The symmetry, B-B bond length shared between a five- and a six-membered ring ($d_{5\text{-}6}$, in Å), B-B bond length shared between two six-membered rings ($d_{6\text{-}6}$, in Å), B-Al bond length ($d_{\text{B-Al}}$, in Å), B-Li bond length ($d_{\text{B-Li}}$, in Å), B_{60} cage diameter (D, in Å) for $Al_{12}Li_{20}$&B_{60} at different levels of theory.

Level	Symm	$d_{5\text{-}6}$	$d_{6\text{-}6}$	$d_{\text{B-Al}}$	$d_{\text{B-Li}}$	D
PBE0/6-31G(d)	I_h	1.788	1.673	2.125	2.207	8.5
PBE0/6-311G(d)	I_h	1.785	1.669	2.124	2.202	8.5
TPSSH/6-31G(d)	I_h	1.793	1.675	2.133	2.219	8.5
B3LYP/6-31G(d)	I_h	1.790	1.677	2.140	2.203	8.5

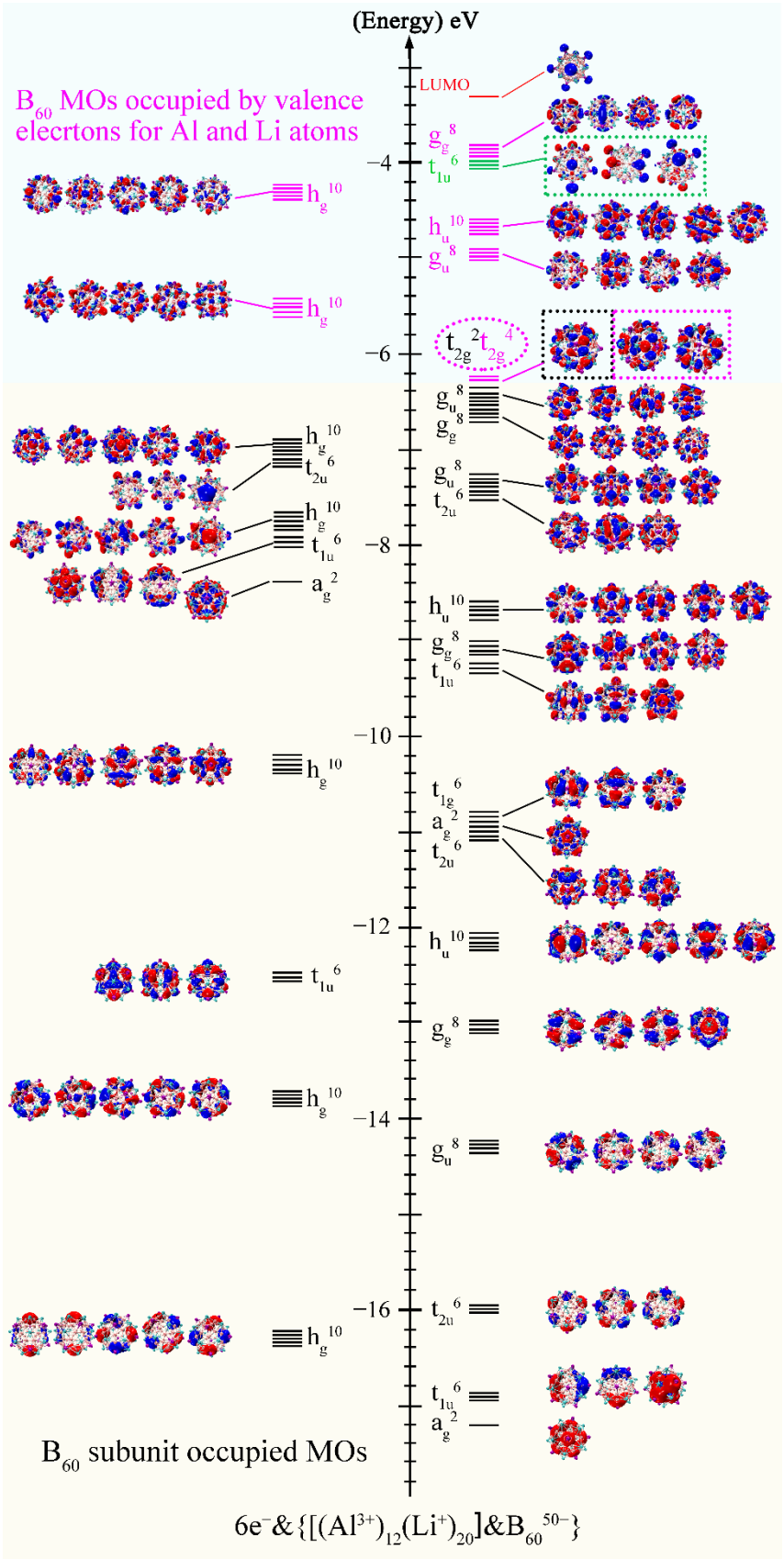

Figure S1. The complete molecular orbital energy diagram of $Al_{12}Li_{20}\&B_{60}$.

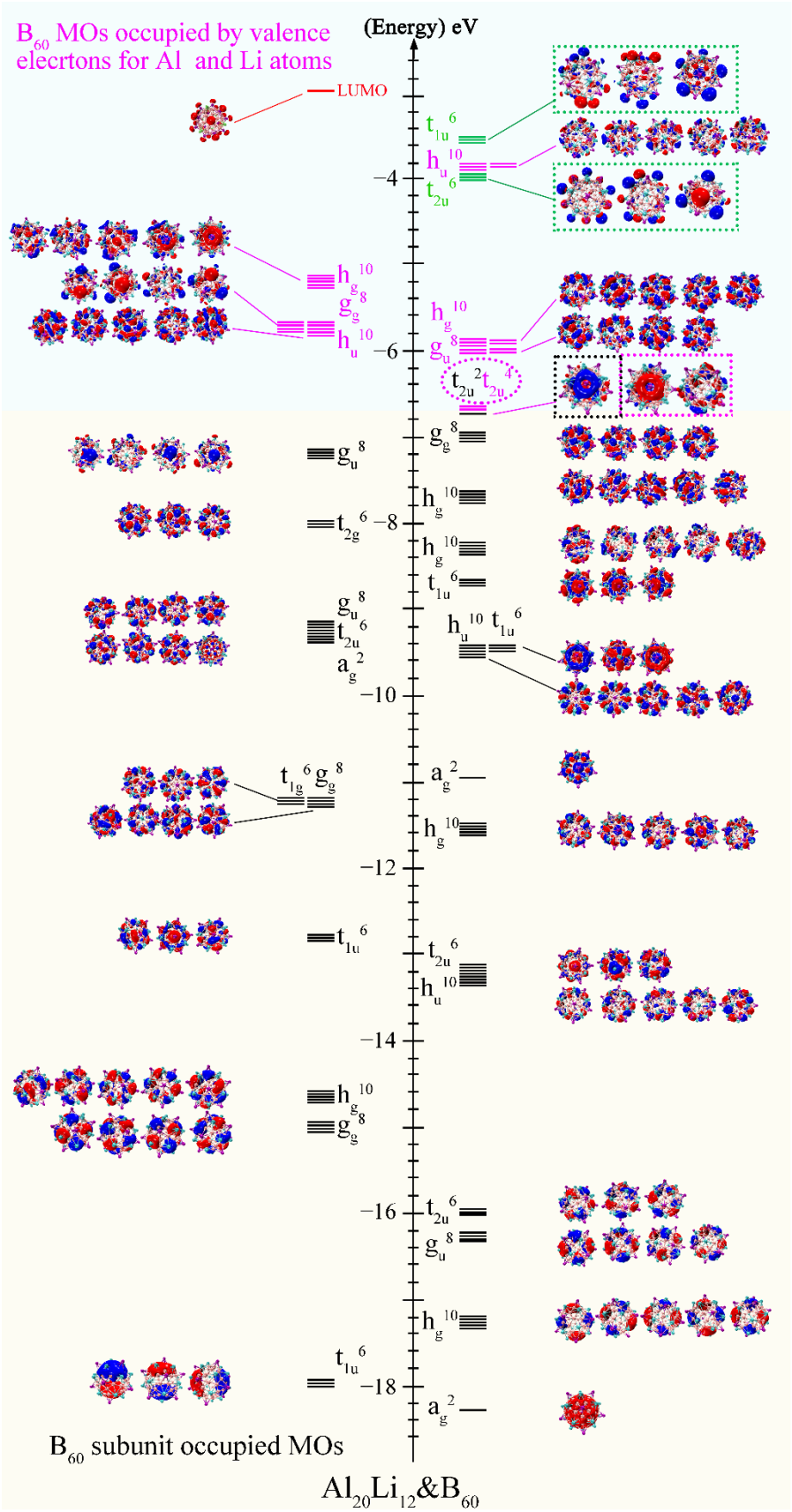

Figure S2. The complete molecular orbital energy diagram of $Al_{20}Li_{12}\&B_{60}$.

Table S2. The push electron oxidation effects of the super-reduced polyanionic state B_{60}^{50-}/B_{60}^{60-} cage with the powerfully strong negative electric fields are characterized as the energies (ΔE) of conversion between unoxidized Ca_6^0 and oxidised Ca_6^{8+}/Ca_6^{10+} in B_{60}^{50-} and B_{60}^{60-} cages, respectively.[a]

System	$V(B_{60})$	Ca_6^0	Ca_6^{10+}	Ca_6^{8+}	ΔE(eV)
$6e^-\&[(Al^{3+})_{12}(Li^+)_{20}]\&B_{60}^{50-}$	−50	−4063.93 a.u.	—	−4058.57 a.u.	145.97
$12e^-\&[(Al^{3+})_{20}(Li^+)_{12}]\&B_{60}^{60-}$	−60	−4063.90 a.u.	−4055.35 a.u.	—	232.58

[a] For $14e^-\&[(Al^{3+})_{12}(Li^+)_{20}]\&[(Ca_6)^{8+}@B_{60}^{50-}]$, the single point energies of the separately neutral Ca_6^0 and Ca_6^{8+} cation were calculated, respectively. Energy difference between the Ca_6^0 and Ca_6^{8+} is 145.97 eV. Similarly, for $22e^-\&[(Al^{3+})_{20}(Li^+)_{12}]\&[(Ca_6)^{10+}@B_{60}^{60-}]$, the single point energy difference value between the neutral Ca_6^0 and Ca_6^{10+} cation is 232.58 eV.

Table S3. The number of excess electron ($N_{\{e\}}$), multiple ionization potentials (IP_n, in eV) for $Al_{12}Li_{20}\&B_{60}$, $Al_{20}Li_{12}\&B_{60}$ and $Al_{12}Li_{20}\&(Ca_6@B_{60})$ as well as $Al_{20}Li_{12}\&(Ca_6@B_{60})$.

System	$N_{\{e\}}$	IP_1	IP_2	IP_3	IP_4	IP_5	IP_6	IP_7	IP_8	IP_9
$6e^-\&[(Al^{3+})_{12}(Li^+)_{20}]\&B_{60}^{50-}$	6	4.63	7.04	8.74	10.98	13.22	15.44			
$12e^-\&[(Al^{3+})_{20}(Li^+)_{12}]\&B_{60}^{60-}$	12	4.25	6.49	8.41	10.54	12.81	14.97	17.39	19.58	21.77
$14e^-\&[(Al^{3+})_{12}(Li^+)_{20}]\&[(Ca_6)^{8+}@B_{60}^{50-}]$	14	4.37	6.26	8.75	10.87	13.24	15.54	17.89	20.10	22.37
$22e^-\&[(Al^{3+})_{20}(Li^+)_{12}]\&[(Ca_6)^{10+}@B_{60}^{60-}]$	22	3.42	6.38	8.26	11.37	13.34	15.12	17.70	19.71	21.35
System	$N_{\{e\}}$	IP_{10}	IP_{11}	IP_{12}	IP_{13}	IP_{14}	IP_{15}	IP_{16}	IP_{17}	IP_{18}
$12e^-\&[(Al^{3+})_{20}(Li^+)_{12}]\&B_{60}^{60-}$	12	24.16	26.32	28.65						
$14e^-\&[(Al^{3+})_{12}(Li^+)_{20}]\&[(Ca_6)^{8+}@B_{60}^{50-}]$	14	24.67	26.70	29.24	31.67	34.08				
$22e^-\&[(Al^{3+})_{20}(Li^+)_{12}]\&[(Ca_6)^{10+}@B_{60}^{60-}]$	22	23.89	25.94	28.73	30.33	33.27	35.00	37.61	39.82	42.14
System	$N_{\{e\}}$	IP_{19}	IP_{20}	IP_{21}	IP_{22}					
$22e^-\&[(Al^{3+})_{20}(Li^+)_{12}]\&[(Ca_6)^{10+}@B_{60}^{60-}]$	22	44.38	46.79	49.06	51.40					

Electrostatic interaction calculation

The ionization potential of an atom can be estimated by the point charge model using Coulomb interaction potential formula as follows:

$$VIP = -k\frac{Qq}{r_q}$$

where k is the correction factor (0.663 for Na, 0.686 for Ti, 0.711 for

$Al_{20}Li_{12}$&(Ca_6@B_{60})), the Q and q denote the charge of nuclear charge (+1) and an electron (−1) for Na and Ti atoms, whereas Q denotes effective nuclear charge (+0.5) for $Al_{20}Li_{12}$&(Ca_6@B_{60}). The r_q denotes the distance between nuclear charge to electron. For example, the estimative VIP_1 values of Na and Ti are 5.14 and 6.83 eV, respectively. The estimative VIP_1 value of $Al_{20}Li_{12}$&(Ca_6@B_{60}) is 3.42 eV.

Cartesian Coordinates

$Al_{12}Li_{20}\&B_{60}$

B	1.44632700	-0.46994000	-4.05212600
B	0.89387900	1.23031900	-4.05212600
B	-3.69400600	-0.32050200	2.23249300
B	-3.17690000	-1.91199000	2.23249300
B	-1.73057400	-2.38193000	3.17237300
B	1.73057400	2.38193000	-3.17237300
B	-2.80012700	0.90981600	3.17237300
B	-0.89387900	-1.23031900	4.05212600
B	3.69400600	0.32050200	-2.23249300
B	-1.44632700	0.46994000	4.05212600
B	3.17690000	1.91199000	-2.23249300
B	0.00000000	1.52075800	4.05212600
B	1.44632700	-3.41416800	-2.23249300
B	2.80012700	-2.43057400	-2.23249300
B	2.80012700	-0.90981600	-3.17237300
B	0.00000000	2.94422800	3.17237300
B	0.00000000	-1.52075800	-4.05212600
B	0.00000000	-2.94422800	-3.17237300
B	-1.44632700	-3.41416800	-2.23249300
B	-2.80012700	2.43057400	2.23249300
B	-1.44632700	-0.46994000	-4.05212600
B	-3.69400600	2.14013500	0.71173500
B	-4.24645400	0.43987600	0.71173500
B	-3.69400600	-2.14013500	-0.71173500
B	-3.17690000	-2.85187000	0.71173500
B	-1.73057400	-3.90268800	0.71173500
B	0.89387900	-1.23031900	4.05212600
B	1.44632700	0.46994000	4.05212600
B	2.80012700	0.90981600	3.17237300
B	0.83669500	-3.61224900	2.23249300
B	-0.83669500	-3.61224900	2.23249300
B	-0.89387900	1.23031900	-4.05212600
B	-1.73057400	2.38193000	-3.17237300
B	-4.24645400	-0.43987600	-0.71173500
B	-3.69400600	0.32050200	-2.23249300
B	-2.80012700	-2.43057400	-2.23249300
B	-2.80012700	-0.90981600	-3.17237300
B	-3.17690000	1.91199000	-2.23249300
B	-3.17690000	2.85187000	-0.71173500
B	-1.73057400	3.90268800	-0.71173500
B	-0.89387900	4.17454700	0.71173500

B	-1.44632700	3.41416800	2.23249300
B	-0.89387900	-4.17454700	-0.71173500
B	0.89387900	-4.17454700	-0.71173500
B	-0.83669500	3.61224900	-2.23249300
B	0.83669500	3.61224900	-2.23249300
B	3.69400600	-0.32050200	2.23249300
B	1.73057400	-2.38193000	3.17237300
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B	1.73057400	-3.90268800	0.71173500
B	3.17690000	-2.85187000	0.71173500
B	3.69400600	-2.14013500	-0.71173500
B	3.17690000	2.85187000	-0.71173500
B	4.24645400	0.43987600	0.71173500
B	3.69400600	2.14013500	0.71173500
B	1.73057400	3.90268800	-0.71173500
B	3.17690000	-1.91199000	2.23249300
B	0.89387900	4.17454700	0.71173500
B	1.44632700	3.41416800	2.23249300
B	2.80012700	2.43057400	2.23249300
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Li	-1.90432400	-2.62107700	-4.24099200
Li	0.00000000	-5.24215400	1.00116200
Li	1.90432400	-2.62107700	-4.24099200
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Li	0.00000000	-3.23982900	4.24099200
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Li	-3.08126100	-1.00116200	4.24099200
Li	-3.08126100	1.00116200	-4.24099200
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Li	-3.08126100	4.24099200	1.00116200
Li	-1.90432400	2.62107700	4.24099200
Li	0.00000000	5.24215400	-1.00116200
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Li	3.08126100	4.24099200	1.00116200
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Li	3.08126100	1.00116200	-4.24099200
Li	4.98558500	-1.61991500	1.00116200
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Al	-4.70895200	-1.53003100	-2.47564300
Al	0.00000000	0.00000000	5.53570500
Al	-2.91029300	-4.00567400	2.47564300

Al	0.00000000	-4.95128500	-2.47564300
Al	4.70895200	-1.53003100	-2.47564300
Al	4.70895200	1.53003100	2.47564300
Al	-2.91029300	4.00567400	-2.47564300
Al	2.91029300	-4.00567400	2.47564300
Al	0.00000000	4.95128500	2.47564300
Al	2.91029300	4.00567400	-2.47564300

$Al_{20}Li_{12}\&B_{60}$

B	0.85774609	1.18058622	4.00473420
B	-0.85774609	1.18058622	4.00473420
B	-0.86407526	-3.55046579	-2.19430508
B	0.86407316	-3.55046710	-2.19430378
B	1.72181736	-2.36988309	-3.09619239
B	-1.72181658	2.36987750	3.09619710
B	-1.72181991	-2.36988179	-3.09619196
B	0.85774609	-1.18058622	-4.00473420
B	0.86407049	3.55046400	2.19430986
B	-0.85774609	-1.18058622	-4.00473420
B	-0.86406960	3.55046419	2.19430989
B	-1.38786233	0.45094381	-4.00473420
B	3.64370430	0.27537475	2.19430989
B	3.10967946	1.91893358	2.19430986
B	1.72181737	2.36987830	3.09619605
B	-2.78596358	0.90521147	-3.09619239
B	1.38786233	-0.45094381	4.00473420
B	2.78595802	-0.90521246	3.09619710
B	2.78595916	-2.36449782	2.19430850
B	-3.10967969	-1.91893867	-2.19430508
B	-0.00000000	-1.45928482	4.00473420
B	-3.10967931	-2.82082331	-0.73502286
B	-1.72181864	-3.82916311	-0.73502286
B	0.85774549	-4.10991713	0.73502518
B	1.72181983	-3.82916329	-0.73501916
B	3.10968078	-2.82082184	-0.73502232
B	1.38786233	0.45094381	-4.00473420
B	-0.00000000	1.45928482	-4.00473420
B	-0.00000154	2.92933159	-3.09619519
B	3.64370815	-0.27537487	-2.19430348
B	3.10967924	-1.91893613	-2.19430794
B	-1.38786233	-0.45094381	4.00473420
B	-2.78595843	-0.90521215	3.09619683
B	-0.85774609	-4.10991725	0.73502380

B	-1.38786200	-3.38027407	2.19430957
B	1.38786117	-3.38027484	2.19430890
B	0.00000059	-2.92932985	3.09619683
B	-2.78595873	-2.36449733	2.19430957
B	-3.64370547	-2.08579929	0.73502380
B	-4.17382140	-0.45426981	0.73502518
B	-4.17382229	0.45427144	-0.73501916
B	-3.64370817	-0.27537227	-2.19430378
B	3.64370489	-2.08579974	0.73502536
B	4.17382134	-0.45427136	0.73502458
B	-3.64370510	0.27537204	2.19430890
B	-3.10967978	1.91893460	2.19430850
B	1.38786368	3.38027500	-2.19430707
B	2.78596037	0.90521178	-3.09619519
B	1.72181547	3.82916409	0.73502519
B	4.17382268	0.45426958	-0.73501806
B	3.64370547	2.08580127	-0.73501817
B	3.10968122	2.82082060	0.73502519
B	-1.72181946	3.82916241	0.73502458
B	0.85774798	4.10991787	-0.73501817
B	-0.85774609	4.10991828	-0.73501806
B	-3.10968017	2.82082171	0.73502536
B	2.78595910	2.36449921	-2.19430707
B	-3.64370520	2.08580028	-0.73502232
B	-2.78596044	2.36449683	-2.19430794
B	-1.38786480	3.38027687	-2.19430348
Al	3.01676871	-4.15222592	0.98020810
Al	1.86446784	-2.56621387	4.15222681
Al	4.88123558	-1.58600723	-0.98020494
Al	3.01676444	0.98020751	4.15222916
Al	4.88123432	1.58600917	0.98020810
Al	3.01677183	-0.98020511	-4.15222436
Al	-0.00000223	-5.13243410	-0.98020494
Al	-0.00000516	-3.17201452	-4.15222896
Al	-1.86446422	-2.56621270	4.15222916
Al	-3.01676872	-4.15222592	0.98020810
Al	-4.88123507	-1.58600752	-0.98020703
Al	-3.01677148	-0.98020747	-4.15222406
Al	-4.88123432	1.58600917	0.98020810
Al	-3.01676988	0.98020698	4.15222534
Al	-1.86446248	2.56621991	-4.15222549
Al	1.86446635	2.56621940	-4.15222406
Al	-3.01676835	4.15222642	-0.98020710
Al	0.00000000	5.13243349	0.98020810

Al	0.00000092	3.17201926	4.15222534
Al	3.01676737	4.15222714	-0.98020703
Li	0.00000000	0.00000000	5.76913888
Li	-3.03301477	-4.17459236	-2.58003169
Li	0.00000206	-5.16007360	2.58003950
Li	-0.00000000	0.00000000	-5.76913888
Li	3.03301477	-4.17459236	-2.58003169
Li	4.90752099	-1.59455239	2.58003950
Li	3.03301683	4.17458603	2.58003950
Li	0.00000333	5.16007751	-2.58003169
Li	-4.90752099	-1.59455239	2.58003950
Li	4.90752637	1.59454848	-2.58003169
Li	-4.90752432	1.59455481	-2.58003169
Li	-3.03301350	4.17458845	2.58003950

$Al_{12}Li_{20}\&(Ca_6@B_{60})$

B	3.85148500	0.12187200	1.72176100
B	2.96456700	0.25433300	3.26912000
B	-3.14369100	2.88829600	-1.55149900
B	-2.23535600	2.86840700	-2.99692000
B	-2.13398700	1.04812400	-3.97113200
B	2.13398700	-1.04812400	3.97113200
B	-3.87825000	1.35984300	-0.88795400
B	-2.96456700	-0.25433300	-3.26912000
B	3.14369100	-2.88829600	1.55149900
B	-3.85148500	-0.12187200	-1.72176100
B	2.23535600	-2.86840700	2.99692000
B	-4.00899500	-1.77051600	-0.83518500
B	3.85148500	0.12187200	-1.72176100
B	3.87825000	-1.35984300	-0.88795400
B	3.87825000	-1.35984300	0.88795400
B	-4.00899500	-1.77051600	0.83518500
B	4.00899500	1.77051600	0.83518500
B	4.00899500	1.77051600	-0.83518500
B	2.94261100	2.96449400	-1.78719700
B	-3.87825000	1.35984300	0.88795400
B	2.94261100	2.96449400	1.78719700
B	-3.14369100	2.88829600	1.55149900
B	-2.41320300	3.49764400	0.00000000
B	0.22581400	4.02871800	-1.46227200
B	-0.48423900	3.36659400	-2.85198600
B	0.59060700	2.12051800	-3.58678900
B	-2.19059800	-1.91576700	-3.09021500
B	-2.94261100	-2.96449400	-1.78719700

B	-1.95560100	-4.07967700	-0.97045100
B	0.37999300	-0.76278100	-4.25091900
B	-0.37999300	0.76278100	-4.25091900
B	2.19059800	1.91576700	3.09021500
B	0.59060700	2.12051800	3.58678900
B	-0.78048900	3.92849300	0.00000000
B	0.22581400	4.02871800	1.46227200
B	1.95560100	4.07967700	-0.97045100
B	1.95560100	4.07967700	0.97045100
B	-0.48423900	3.36659400	2.85198600
B	-2.23535600	2.86840700	2.99692000
B	-2.13398700	1.04812400	3.97113200
B	-2.96456700	-0.25433300	3.26912000
B	-3.85148500	-0.12187200	1.72176100
B	2.19059800	1.91576700	-3.09021500
B	2.96456700	0.25433300	-3.26912000
B	-0.37999300	0.76278100	4.25091900
B	0.37999300	-0.76278100	4.25091900
B	-0.22581400	-4.02871800	-1.46227200
B	-0.59060700	-2.12051800	-3.58678900
B	2.41320300	-3.49764400	0.00000000
B	2.13398700	-1.04812400	-3.97113200
B	2.23535600	-2.86840700	-2.99692000
B	3.14369100	-2.88829600	-1.55149900
B	0.48423900	-3.36659400	2.85198600
B	0.78048900	-3.92849300	0.00000000
B	-0.22581400	-4.02871800	1.46227200
B	-0.59060700	-2.12051800	3.58678900
B	0.48423900	-3.36659400	-2.85198600
B	-2.19059800	-1.91576700	3.09021500
B	-2.94261100	-2.96449400	1.78719700
B	-1.95560100	-4.07967700	0.97045100
Li	1.62323300	4.11805200	-3.16837700
Li	3.98003600	3.86038600	0.00000000
Li	1.73978000	0.84540800	-5.04003000
Li	5.29835100	0.19152700	0.00000000
Li	4.12740400	-1.65743900	-3.12891800
Li	-1.73978000	-0.84540800	-5.04003000
Li	-1.88626800	4.73985100	-1.81380700
Li	-4.12740400	1.65743900	-3.12891800
Li	1.62323300	4.11805200	3.16837700
Li	-1.88626800	4.73985100	1.81380700
Li	-4.12740400	1.65743900	3.12891800
Li	-5.29835100	-0.19152700	0.00000000

Li	-1.73978000	-0.84540800	5.04003000
Li	1.73978000	0.84540800	5.04003000
Li	-3.98003600	-3.86038600	0.00000000
Li	-1.62323300	-4.11805200	-3.16837700
Li	-1.62323300	-4.11805200	3.16837700
Li	1.88626800	-4.73985100	1.81380700
Li	4.12740400	-1.65743900	3.12891800
Li	1.88626800	-4.73985100	-1.81380700
Al	4.35184500	1.83723500	2.92250200
Al	-4.57015300	3.24495600	0.00000000
Al	0.71811400	5.57234900	0.00000000
Al	-4.35184500	-1.83723500	-2.92250200
Al	-1.09886200	2.70443500	-4.76593200
Al	4.35184500	1.83723500	-2.92250200
Al	4.57015300	-3.24495600	0.00000000
Al	-0.71811400	-5.57234900	0.00000000
Al	-1.09886200	2.70443500	4.76593200
Al	1.09886200	-2.70443500	-4.76593200
Al	-4.35184500	-1.83723500	2.92250200
Al	1.09886200	-2.70443500	4.76593200
Ca	1.21414600	-1.09756700	-1.63124300
Ca	-1.21414600	1.09756700	1.63124300
Ca	1.48932000	1.77999200	0.00000000
Ca	-1.48932000	-1.77999200	0.00000000
Ca	1.21414600	-1.09756700	1.63124300
Ca	-1.21414600	1.09756700	-1.63124300

$Al_{20}Li_{12}$&(Ca_6@B_{60})

B	-3.74245600	-1.74144000	1.37066000
B	-2.69556200	-3.07290500	0.83990800
B	1.74144000	1.37066000	-3.74245600
B	0.83990800	2.69556200	-3.07290500
B	1.37066000	3.74245600	-1.74144000
B	-1.37066000	-3.74245600	1.74144000
B	3.07290500	0.83990800	-2.69556200
B	2.69556200	3.07290500	-0.83990800
B	-1.74144000	-1.37066000	3.74245600
B	3.74245600	1.74144000	-1.37066000
B	-0.83990800	-2.69556200	3.07290500
B	4.52482800	0.93578300	0.00000000
B	-3.74245600	1.74144000	1.37066000
B	-3.07290500	0.83990800	2.69556200
B	-3.07290500	-0.83990800	2.69556200
B	4.52482800	-0.93578300	0.00000000

B	-4.52482800	-0.93578300	0.00000000
B	-4.52482800	0.93578300	0.00000000
B	-3.74245600	1.74144000	-1.37066000
B	3.07290500	-0.83990800	-2.69556200
B	-3.74245600	-1.74144000	-1.37066000
B	1.74144000	-1.37066000	-3.74245600
B	0.93578300	0.00000000	-4.52482800
B	-1.74144000	1.37066000	-3.74245600
B	-0.83990800	2.69556200	-3.07290500
B	-1.37066000	3.74245600	-1.74144000
B	2.69556200	3.07290500	0.83990800
B	3.74245600	1.74144000	1.37066000
B	3.07290500	0.83990800	2.69556200
B	0.00000000	4.52482800	0.93578300
B	0.00000000	4.52482800	-0.93578300
B	-2.69556200	-3.07290500	-0.83990800
B	-1.37066000	-3.74245600	-1.74144000
B	-0.93578300	0.00000000	-4.52482800
B	-1.74144000	-1.37066000	-3.74245600
B	-3.07290500	0.83990800	-2.69556200
B	-3.07290500	-0.83990800	-2.69556200
B	-0.83990800	-2.69556200	-3.07290500
B	0.83990800	-2.69556200	-3.07290500
B	1.37066000	-3.74245600	-1.74144000
B	2.69556200	-3.07290500	-0.83990800
B	3.74245600	-1.74144000	-1.37066000
B	-2.69556200	3.07290500	-0.83990800
B	-2.69556200	3.07290500	0.83990800
B	0.00000000	-4.52482800	-0.93578300
B	0.00000000	-4.52482800	0.93578300
B	1.74144000	1.37066000	3.74245600
B	1.37066000	3.74245600	1.74144000
B	-0.93578300	0.00000000	4.52482800
B	-1.37066000	3.74245600	1.74144000
B	-0.83990800	2.69556200	3.07290500
B	-1.74144000	1.37066000	3.74245600
B	0.83990800	-2.69556200	3.07290500
B	0.93578300	0.00000000	4.52482800
B	1.74144000	-1.37066000	3.74245600
B	1.37066000	-3.74245600	1.74144000
B	0.83990800	2.69556200	3.07290500
B	2.69556200	-3.07290500	0.83990800
B	3.74245600	-1.74144000	1.37066000
B	3.07290500	-0.83990800	2.69556200

Al	-3.03564000	3.03564000	-3.03564000
Al	-5.07740000	0.00000000	-1.99184700
Al	-1.99184700	5.07740000	0.00000000
Al	-5.07740000	0.00000000	1.99184700
Al	-3.03564000	3.03564000	3.03564000
Al	1.99184700	5.07740000	0.00000000
Al	0.00000000	1.99184700	-5.07740000
Al	3.03564000	3.03564000	-3.03564000
Al	-3.03564000	-3.03564000	-3.03564000
Al	0.00000000	-1.99184700	-5.07740000
Al	3.03564000	-3.03564000	-3.03564000
Al	5.07740000	0.00000000	-1.99184700
Al	1.99184700	-5.07740000	0.00000000
Al	-1.99184700	-5.07740000	0.00000000
Al	5.07740000	0.00000000	1.99184700
Al	3.03564000	3.03564000	3.03564000
Al	3.03564000	-3.03564000	3.03564000
Al	0.00000000	-1.99184700	5.07740000
Al	-3.03564000	-3.03564000	3.03564000
Al	0.00000000	1.99184700	5.07740000
Li	-4.83520400	-3.21277400	0.00000000
Li	3.21277400	0.00000000	-4.83520400
Li	-3.21277400	0.00000000	-4.83520400
Li	4.83520400	3.21277400	0.00000000
Li	0.00000000	4.83520400	-3.21277400
Li	-4.83520400	3.21277400	0.00000000
Li	-3.21277400	0.00000000	4.83520400
Li	3.21277400	0.00000000	4.83520400
Li	0.00000000	-4.83520400	-3.21277400
Li	0.00000000	4.83520400	3.21277400
Li	4.83520400	-3.21277400	0.00000000
Li	0.00000000	-4.83520400	3.21277400
Ca	0.00000000	0.00000000	2.26090400
Ca	0.00000000	0.00000000	-2.26090400
Ca	0.00000000	2.26090400	0.00000000
Ca	0.00000000	-2.26090400	0.00000000
Ca	2.26090400	0.00000000	0.00000000
Ca	-2.26090400	0.00000000	0.00000000