

Electronic Supporting Information

Structure and Stability of Aluminum Doped Lithium Clusters

(Li_nAl^{0/+}, n = 1 - 8): A Case of the Phenomenological Shell Model

Truong Ba Tai, Pham Vu Nhat and Minh Tho Nguyen

Table 1. The total energy E , zero point energies (ZPE) and relative energies (ΔE) of all isomers using the B3LYP/aug-cc-pVTZ level.

Structures	E	ZPE	ΔE
LiAl (¹ Σ^+)	-249.9156285	0.0006920	0.00
LiAl (³ Σ_g^+)	-249.9083532	0.0007460	4.60
Li ₂ Al-I (C _{2v} , ² B ₂)	-257.4457577	0.0017501	0.00
Li ₂ Al-II (² Σ^+)	-257.4455293	0.0017132	0.12
Li ₂ Al-III (C _{2v} , ² A ₁)	-257.4366085	0.0020015	5.90
Li ₂ Al-II (² Σ^+)	-257.4253162	0.0016246	12.75
Li ₃ Al-I (C _{2v} , ¹ A ₁)	-264.9893279	0.0032495	0.00
Li ₃ Al-II (D _{3h} , ¹ A ₁ ')	-264.9771896	0.0028200	7.35
Li ₃ Al-III (C _{3v} , ³ A ₁)	-264.9865588	0.0033714	1.81
Li ₃ Al-IV (C _{2v} , ³ B ₂)	-264.9526748	0.0023597	22.44
Li ₄ Al-I (C _{2v} , ² B ₂)	-272.5344883	0.0049952	0.00
Li ₄ Al-II (C _{4v} , ² A ₁)	-272.5254194	0.0044913	5.37
Li ₄ Al-III (D _{4h} , ² A _{2u})	-272.5212557	0.0041636	7.78
Li ₄ Al-IV (C _{3v} , ⁴ A ₁)	-272.5100645	0.0047590	15.18
Li ₄ Al-V (C _{2v} , ⁴ A ₂)	-272.4930018	0.0039015	25.35
Li ₅ Al-I (C _{4v} , ¹ A ₁)	-280.0864923	0.0066948	0.00
Li ₅ Al-II (C _s , ³ A')	-280.0590508	0.0060262	16.80

Li₆Al-I ($C_s, {}^2A'$)	-287.6145639	0.0075656	0.00
Li₆Al-II ($C_{5v}, {}^2A_1$)	-287.6119324	0.0074678	1.60
Li₆Al-III ($O_h, {}^2A_{1g}$)	-287.6094412	0.0060032	2.23
Li₇Al-I ($C_s, {}^1A'$)	-295.1461407	0.0086901	0.81
Li₇Al-II ($C_s, {}^1A'$)	-295.1479198	0.0091747	0.00
Li₇Al-III ($C_s, {}^1A'$)	-295.146041	0.0088299	0.96
Li₇Al-V ($C_{3v}, {}^1A_1$)	-295.1446743	0.0079845	1.29
Li₇Al-VI ($C_{2v}, {}^1A_1$)	-295.1454135	0.0083970	1.08
Li₈Al-I ($C_{2v}, {}^2A_1$)	-302.6742371	0.0099649	0.76
Li₈Al-II ($C_s, 2A'$)	-302.6757579	0.0102692	0.00

LiAl (${}^2\Sigma^+$)	-249.7229883	0.0005060	0.00
Li₂Al-Ic (${}^1\Sigma_g^+$)	-257.2872655	0.0021349	0.00
Li₂Al-IIc ($C_{2v}, {}^1A_1$)	-257.2590054	0.0014707	17.32
Li₃Al-Ic ($C_{2v}, {}^2B_2$)	-264.8226129	0.0030767	0.00
Li₃Al-IIc ($C_{2v}, {}^2A_1$)	-264.8188146	0.0027070	2.15
Li₃Al-IIIc ($C_{3v}, {}^2A_1$)	-264.7983692	0.0024157	14.80
Li₄Al-Ic ($D_{4h}, {}^1A_{1g}$)	-272.3761812	0.0043954	0.00
Li₄Al-IIc ($C_{2v}, {}^1A_1$)	-272.3553701	0.0040422	12.84
Li₄Al-IIIc ($C_{3v}, {}^1A_1$)	-272.340714	0.0039800	22.00
Li₅Al-Ic ($C_{4v}, {}^2A_1$)	-279.9169918	0.0053420	0.00
Li₅Al-IIc ($C_s, {}^2A'$)	-279.9172865	0.0056587	0.00
Li₆Al-Ic ($O_h, {}^1A_{1g}$)	-287.478723	0.0070690	0.00
Li₆Al-IIc ($C_{5v}, {}^1A_1$)	-287.4680624	0.0078527	7.18
Li₇Al-Ic ($D_{5h}, {}^2A_1'$)	-294.9999309	0.0066507	0.45
Li₇Al-IIc ($C_{3v}, {}^2A_1$)	-295.0019556	0.0080228	0.04
Li₇Al-IIIc ($C_{2v}, {}^2A_1$)	-295.0023913	0.0083974	0.00

Li₈Al-Ic ($C_{3v}, ^1A_1$)	-302.5430025	0.0105066	0.00
Li₈Al-IIc ($D_{2d}, ^1A_1$)	-302.5303711	0.0093922	7.23




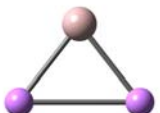
Table S2. Total energy of the global minimum $Li_nAl^{0/+}$ using the CCSD(T)/aug-cc-pVaZ (a = D, T, Q) level and Extrapolated CBS energies.


Total energies, a.u	
LiAl ($C_{\infty h}, ^1\Sigma^+$)	
CCSD(T)/aug-cc-pVDZ	-249.388712
CCSD(T)/aug-cc-pVTZ	-249.401466
CCSD(T)/aug-cc-pVQZ	-249.404596
CBS	-249.40627
Li₂Al-I ($C_{2v}, ^2B_2$)	
CCSD(T)/aug-cc-pVDZ	-256.863452
CCSD(T)/aug-cc-pVTZ	-256.878776
CCSD(T)/aug-cc-pVQZ	-256.882479
CBS	-256.88445
Li₃Al-I ($C_{2v}, ^1A_1$)	
CCSD(T)/aug-cc-pVDZ	-264.346204
CCSD(T)/aug-cc-pVTZ	-264.365479
CCSD(T)/aug-cc-pVQZ	-264.370111
CBS	-264.37257
Li₄Al-I ($C_{2v}, ^2B_2$)	


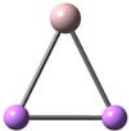
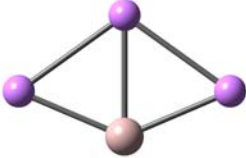
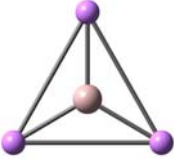
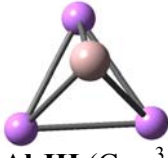
CCSD(T)/aug-cc-pVDZ	-271.834099
CCSD(T)/aug-cc-pVTZ	-271.856894
CCSD(T)/aug-cc-pVQZ	-271.862237
CBS	-271.86506
Li₅Al-I (C_{4v}, ¹A₁)	
CCSD(T)/aug-cc-pVDZ	-279.332100
CCSD(T)/aug-cc-pVTZ	-279.358101
CCSD(T)/aug-cc-pVQZ	-279.364254
CBS	-279.36751
LiAl (²Σ⁺)	
CCSD(T)/aug-cc-pVDZ	-249.200597
CCSD(T)/aug-cc-pVTZ	-249.210374
CCSD(T)/aug-cc-pVQZ	-249.212868
CBS	-249.21421
Li₂Al-Ic (¹Σ⁺_g)	
CCSD(T)/aug-cc-pVDZ	-256.705465
CCSD(T)/aug-cc-pVTZ	-256.721269
CCSD(T)/aug-cc-pVQZ	-256.724893
CBS	-256.72679
Li₃Al-Ic (C_{2v}, ²B₂)	
CCSD(T)/aug-cc-pVDZ	-264.180874
CCSD(T)/aug-cc-pVTZ	-264.199647
CCSD(T)/aug-cc-pVQZ	-264.20406
CBS	-264.20639
Li₄Al-Ic (D_{4h}, ¹A_{1g})	
CCSD(T)/aug-cc-pVDZ	-271.675851
CCSD(T)/aug-cc-pVTZ	-271.699383

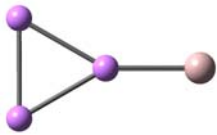
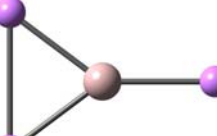
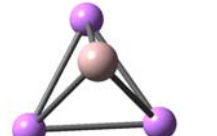

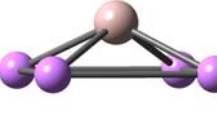
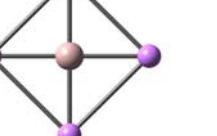
CCSD(T)/aug-cc-pVQZ	-271.704856
CBS	-271.70774
Li₅Al-IIc (C_s, ²A')	
CCSD(T)/aug-cc-pVDZ	-279.161104
CCSD(T)/aug-cc-pVTZ	-279.186892
CCSD(T)/aug-cc-pVQZ	-279.192979
CBS	-279.1962
Li₆Al-I (C_s, ²A')	
CCSD(T)/aug-cc-pVDZ	-286.801025
CCSD(T)/aug-cc-pVTZ	-286.829749
Li₆Al-Ic (O_h, ¹A_{1g})	
CCSD(T)/aug-cc-pVDZ	-286.667688
CCSD(T)/aug-cc-pVTZ	-286.697292
Li₇Al-II (C_s, ¹A')	
CCSD(T)/aug-cc-pVDZ	-294.278642
CCSD(T)/aug-cc-pVTZ	-294.309581
Li₇Al-IIc (C_{3v}, ²A₁)	
CCSD(T)/aug-cc-pVDZ	-294.132668
CCSD(T)/aug-cc-pVTZ	-294.163336
Li₈Al-I (C_{2v}, ²A₁)	
CCSD(T)/aug-cc-pVDZ	-301.7493998
CCSD(T)/aug-cc-pVTZ	-301.782728
Li₈Al-Ic (C_{3v}, ¹A₁)	
CCSD(T)/aug-cc-pVDZ	-301.617740
CCSD(T)/aug-cc-pVTZ	-301.6505092


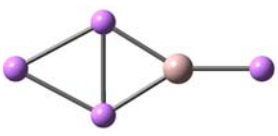
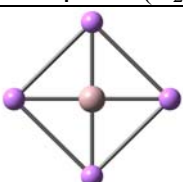
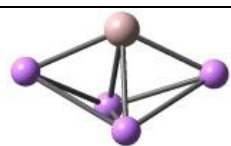
Table S3. Coordinates of all isomers using the B3LYP/aug-cc-pVTZ level.

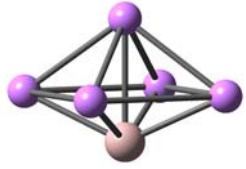
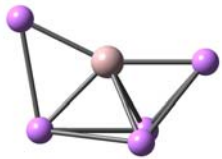
Structure	Cartesian coordinates			
 LiAl ($^1\Sigma^+$)	Li	0.00000000	0.00000000	-2.34472300
	Al	0.00000000	0.00000000	0.54109000
 LiAl ($^3\Sigma^-$)	Li	0.00000000	0.00000000	-2.14438300
	Al	0.00000000	0.00000000	0.49485800
 LiAl⁺ ($^2\Sigma^+$)	Li	0.00000000	0.00000000	-2.46872400
	Al	0.00000000	0.00000000	0.56970600
 Li₂Al-I ($C_{2v}, ^2B_2$)	Li	0.00000000	1.56359300	-1.38235500
	Al	0.00000000	0.00000000	0.63801000
	Li	0.00000000	-1.56359300	-1.38235500
Li₂Al-II ($^2\Sigma^+$)	Al	0.00000000	0.12950100	0.00000000
	Li	2.59256900	-0.28058900	0.00000000
	Li	-2.59256900	-0.28058100	0.00000000

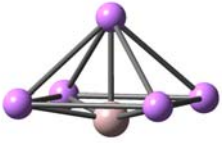
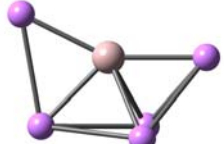
 <p>Li₂Al-III ($C_{2v}, {}^2A_1$)</p>	Li	0.00000000	2.54621600	-0.49248400
	Al	0.00000000	0.00000000	0.22730000
	Li	0.00000000	-2.54621600	-0.49248400
<p>Li₂Al-IV (${}^2\Sigma_g^+$)</p>	Al	0.00000000	0.00000000	1.45637132
	Li	0.00000000	0.00000000	-1.60434168
	Li	0.00000000	0.00000000	-4.70660068

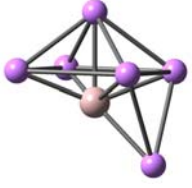

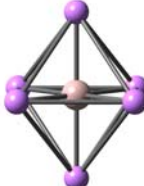
 <p>Li₂Al-Ic (${}^1\Sigma_g^+$)</p>	Al	0.00000000	0.00000000	0.00000000
	Li	0.00000000	0.00000000	2.75400200
	Li	0.00000000	0.00000000	-2.75400200
 <p>Li₂Al-IIc ($C_{2v}, {}^1A_1$)</p>	Li	0.00000000	1.42498900	-2.01039400
	Al	0.00000000	0.00000000	0.92787400
	Li	0.00000000	-1.42498900	-2.01039400
 <p>Li₃Al-I ($C_{2v}, {}^1A_1$)</p>	Li	0.00000000	-2.47969589	-0.38248610
	Li	-0.00000000	2.47969589	-0.38248610
	Li	0.00000000	0.00000000	-2.16245727
	Al	0.00000000	0.00000000	0.67556073
 <p>Li₃Al-II ($D_{3h}, {}^1A_1'$)</p>	Al	0.00000000	0.00000000	0.00000000
	Li	0.00000000	2.63625100	0.00000000
	Li	2.28306000	-1.31812500	0.00000000
	Li	-2.28306000	-1.31812500	0.00000000
 <p>Li₃Al-III ($C_{3v}, {}^3A_1$)</p>	Al	0.00000000	0.00000000	0.88344800
	Li	0.00000000	1.67074800	-1.27609200
	Li	-1.44691000	-0.83537400	-1.27609200
	Li	1.44691000	-0.83537400	-1.27609200

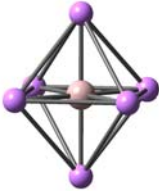
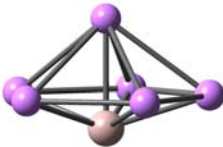
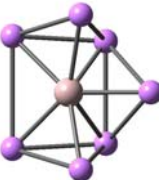
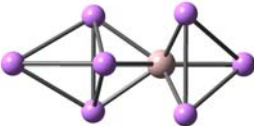
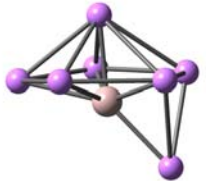

 <p>Li₃Al-IV (C_{2v}, 3B_2)</p>	<p>Li 0.00000000 1.43877800 -3.40456800 Li 0.00000000 -1.43877800 -3.40456800 Li 0.00000000 0.00000000 -0.92164800 Al 0.00000000 0.00000000 1.78402700</p>
 <p>Li₃Al-Ic (C_{2v}, 2B_2)</p>	<p>Al 0.00000000 0.00000000 0.23004000 Li 0.00000000 0.00000000 2.88623700 Li 0.00000000 1.63529200 -1.94153900 Li 0.00000000 -1.63529200 -1.94153900</p>
 <p>Li₃Al-IIIc (C_{3v}, 4A_1)</p>	<p>Al 0.00000000 -0.00000000 0.61671600 Li 0.00000000 2.18242688 -0.89081262 Li -1.89003712 -1.09121344 -0.89081262 Li 1.89003712 -1.09121344 -0.89081262</p>
 <p>Li₄Al-I (C_{2v}, 2B_2)</p>	<p>Li 0.00000000 1.39388800 -1.48731388 Li 2.41483100 -0.00000000 -0.29696888 Li -2.41483100 -0.00000000 -0.29696888 Li 0.00000000 -1.39388800 -1.48731388 Al 0.00000000 0.00000000 0.82351512</p>
 <p>Li₄Al-II (C_{4v}, 2A_1)</p>	<p>Li 0.00000000 2.36335700 -0.52045800 Li 2.36335500 0.00000000 -0.52046000 Li -2.36335500 0.00000000 -0.52046000 Li 0.00000000 -2.36335700 -0.52045800 Al 0.00000000 0.00000000 0.48042400</p>
 <p>Li₄Al-III (D_{4h}, $^2A_{2u}$)</p>	<p>Li 0.00000000 2.50880600 0.00000000 Li 2.50880600 0.00000000 0.00000000 Li 0.00000000 -2.50880600 0.00000000 Li -2.50880600 0.00000000 0.00000000 Al 0.00000000 0.00000000 0.00000000</p>

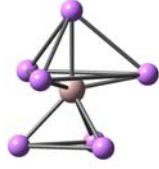
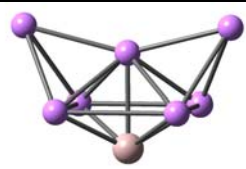
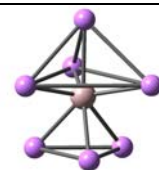
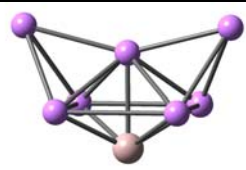
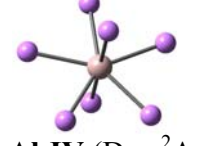
 <p>Li₄Al-IV ($C_{3v}, {}^4A_1$)</p>	Li 0.00000000 1.60425900 -0.83716200 Li -1.38932900 -0.80212900 -0.83716200 Li 1.38932900 -0.80212900 -0.83716200 Al 0.00000000 0.00000000 1.37423600 Li 0.00000000 0.00000000 -3.44353700
 <p>Li₄Al-V ($C_{2v}, {}^4A_2$)</p>	Li -1.39016900 -1.43394400 0.00000000 Li 1.39096800 -1.43352700 0.00000000 Li 0.00173500 -4.07893200 0.00000000 Al 0.00000000 0.82828500 0.00000000 Li -0.00253400 3.35716900 0.00000000
 <p>Li₄Al-Ic ($D_{4h}, {}^1A_{1g}$)</p>	Li 0.00000000 2.61733500 0.00000000 Li 2.61733500 0.00000000 0.00000000 Li 0.00000000 -2.61733500 0.00000000 Li -2.61733500 0.00000000 0.00000000 Al 0.00000000 0.00000000 0.00000000
	Li -0.00000700 1.74683300 -1.33540000 Li -2.58636800 0.04748300 -0.00000800 Li 2.58636800 0.04748300 -0.00001500 Li 0.00000700 1.74285200 1.33747600 Al 0.00000000 -0.82722700 -0.00047400

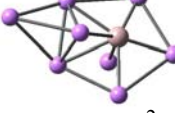
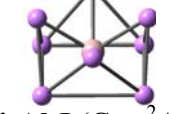
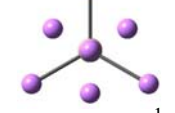
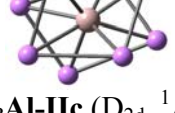
 <p>Li₅Al-I ($C_{4v}, {}^1A_1$)</p>	Al -0.00000400 0.00000000 -0.75919000 Li 0.02510300 -2.36107100 0.32065400 Li 2.36107000 0.02509300 0.32065000 Li -0.02508400 2.36107200 0.32065400 Li 0.00000000 0.00000000 2.00720800 Li -2.36107300 -0.02509300 0.32065700
 <p>Li₅Al-II ($C_s, {}^3A'$)</p>	Al -0.21585400 -0.46478600 -0.00000100 Li -1.29495900 1.93300800 0.00000200 Li -2.85647100 -0.74974600 0.00000100 Li 2.28559200 -1.39758000 0.00000200 Li 1.40060300 1.11419400 1.38372900 Li 1.40060200 1.11419700 -1.38372800

 <p>Li₅Al-Ic ($C_{4v}, ^2A_1$)</p>	<table border="1"> <tbody> <tr><td>Al</td><td>0.00000000</td><td>0.00000000</td><td>0.45573600</td></tr> <tr><td>Li</td><td>0.00000000</td><td>0.00000000</td><td>-2.03804700</td></tr> <tr><td>Li</td><td>0.00000000</td><td>2.54846800</td><td>0.01579800</td></tr> <tr><td>Li</td><td>2.54846800</td><td>0.00000000</td><td>0.01579800</td></tr> <tr><td>Li</td><td>-2.54846800</td><td>0.00000000</td><td>0.01579800</td></tr> <tr><td>Li</td><td>0.00000000</td><td>-2.54846800</td><td>0.01579800</td></tr> </tbody> </table>	Al	0.00000000	0.00000000	0.45573600	Li	0.00000000	0.00000000	-2.03804700	Li	0.00000000	2.54846800	0.01579800	Li	2.54846800	0.00000000	0.01579800	Li	-2.54846800	0.00000000	0.01579800	Li	0.00000000	-2.54846800	0.01579800
Al	0.00000000	0.00000000	0.45573600																						
Li	0.00000000	0.00000000	-2.03804700																						
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Al	-0.21585400	-0.46478600	-0.00000100																						
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Structure	Coordinates																												
 <p>Li₆Al-I ($C_s, ^2A'$)</p>	<table border="1"> <tbody> <tr><td>Li</td><td>-1.91916800</td><td>-1.65664800</td><td>-0.59200900</td></tr> <tr><td>Li</td><td>-1.33529500</td><td>-0.00016500</td><td>1.76956000</td></tr> <tr><td>Li</td><td>1.15166100</td><td>1.57879300</td><td>1.23413100</td></tr> <tr><td>Li</td><td>2.63031700</td><td>0.00023800</td><td>-1.00272000</td></tr> <tr><td>Li</td><td>1.15242000</td><td>-1.57886100</td><td>1.23489800</td></tr> <tr><td>Li</td><td>-1.91500400</td><td>1.65993200</td><td>-0.59067600</td></tr> <tr><td>Al</td><td>0.05424700</td><td>-0.00075900</td><td>-0.47381200</td></tr> </tbody> </table>	Li	-1.91916800	-1.65664800	-0.59200900	Li	-1.33529500	-0.00016500	1.76956000	Li	1.15166100	1.57879300	1.23413100	Li	2.63031700	0.00023800	-1.00272000	Li	1.15242000	-1.57886100	1.23489800	Li	-1.91500400	1.65993200	-0.59067600	Al	0.05424700	-0.00075900	-0.47381200
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Al	0.05424700	-0.00075900	-0.47381200																										
 <p>Li₆Al-II ($C_{5v}, ^2A_1$)</p>	<table border="1"> <tbody> <tr><td>Al</td><td>0.00000000</td><td>0.00000000</td><td>0.66835000</td></tr> <tr><td>Li</td><td>0.00000000</td><td>2.51403900</td><td>-0.18574300</td></tr> <tr><td>Li</td><td>2.39099300</td><td>0.77688100</td><td>-0.18574300</td></tr> <tr><td>Li</td><td>1.47771500</td><td>-2.03390000</td><td>-0.18574300</td></tr> <tr><td>Li</td><td>-2.39099300</td><td>0.77688100</td><td>-0.18574300</td></tr> <tr><td>Li</td><td>-1.47771500</td><td>-2.03390000</td><td>-0.18574300</td></tr> <tr><td>Li</td><td>0.00000000</td><td>0.00000000</td><td>-1.96746900</td></tr> </tbody> </table>	Al	0.00000000	0.00000000	0.66835000	Li	0.00000000	2.51403900	-0.18574300	Li	2.39099300	0.77688100	-0.18574300	Li	1.47771500	-2.03390000	-0.18574300	Li	-2.39099300	0.77688100	-0.18574300	Li	-1.47771500	-2.03390000	-0.18574300	Li	0.00000000	0.00000000	-1.96746900
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Li	0.00000000	0.00000000	-1.96746900																										
 <p>Li₆Al-III ($O_h, ^2A_{1g}$)</p>	<table border="1"> <tbody> <tr><td>Li</td><td>0.00000000</td><td>0.00000000</td><td>2.50183600</td></tr> <tr><td>Li</td><td>0.00000000</td><td>2.50183600</td><td>0.00000000</td></tr> <tr><td>Li</td><td>0.00000000</td><td>0.00000000</td><td>-2.50183600</td></tr> <tr><td>Li</td><td>2.50183600</td><td>0.00000000</td><td>0.00000000</td></tr> <tr><td>Li</td><td>0.00000000</td><td>-2.50183600</td><td>0.00000000</td></tr> <tr><td>Li</td><td>-2.50183600</td><td>0.00000000</td><td>0.00000000</td></tr> <tr><td>Al</td><td>0.00000000</td><td>0.00000000</td><td>0.00000000</td></tr> </tbody> </table>	Li	0.00000000	0.00000000	2.50183600	Li	0.00000000	2.50183600	0.00000000	Li	0.00000000	0.00000000	-2.50183600	Li	2.50183600	0.00000000	0.00000000	Li	0.00000000	-2.50183600	0.00000000	Li	-2.50183600	0.00000000	0.00000000	Al	0.00000000	0.00000000	0.00000000
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Al	0.00000000	0.00000000	0.00000000																										

 <p>Li₆Al-Ic (O_h, $^1A_{1g}$)</p>	Li 0.00000000 0.00000000 2.51180300 Li 0.00000000 2.51180300 0.00000000 Li 0.00000000 0.00000000 -2.51180300 Li 2.51180300 0.00000000 0.00000000 Li 0.00000000 -2.51180300 0.00000000 Li -2.51180300 0.00000000 0.00000000 Al 0.00000000 0.00000000 0.00000000
 <p>Li₆Al-IIc (C_{5v}, 1A_1)</p>	Al -0.00005600 0.00004800 -0.64729700 Li 2.21645800 -1.24448200 0.14824900 Li 1.86851800 1.72333800 0.14960700 Li -1.06125500 2.30982100 0.14932600 Li -0.49905600 -2.49233900 0.14912100 Li -2.52484100 -0.29536300 0.14902300 Li 0.00042000 -0.00118200 2.05962600
 <p>Li₇Al-I (C_s, 1A_1)</p>	Li -0.03655518 2.04061185 -1.73956212 Li 1.20787566 -0.63498472 2.39112150 Li -0.03655518 2.04061185 1.73956212 Li -1.73120677 -0.39000072 -1.58016892 Li -1.73120677 -0.39000072 1.58016892 Li 1.20787566 -0.63498472 -2.39112150 Li -0.08659746 -2.44757383 0.00000000 Al 0.27775714 0.09552708 0.00000000
 <p>Li₇Al-II (C_s, 1A_1)</p>	Li 0.00623589 -1.08041280 2.36516038 Li 0.00623589 -1.08041280 -2.36516038 Al 0.39439402 0.02525692 0.00000000 Li -1.08048302 1.67097079 1.40827021 Li 0.85119468 -2.67997297 0.00000000 Li -1.08048302 1.67097079 -1.40827021 Li 1.48438342 2.51349618 0.00000000 Li -1.89606470 -1.12414863 0.00000000
 <p>Li₇Al-III (C_s, 1A_1)</p>	Li 1.08041300 2.36516000 -0.00623500 Li 1.08036100 -2.36517800 -0.00621400 Al -0.02525700 -0.00000100 -0.39439400 Li -1.67097100 1.40827000 1.08048300 Li 2.67997300 -0.00002500 -0.85119400 Li -1.67098300 -1.40821800 1.08052000 Li -2.51349600 -0.00001100 -1.48438400 Li 1.12414800 0.00000400 1.89606500
	Li 0.00000000 -2.66226500 -0.00000000 Li -0.00000000 -0.00000000 -2.56996000 Li 0.00000000 -0.00000000 2.56996000 Li -2.53196448 -0.82268513 -0.00000000 Li 2.53196448 -0.82268513 -0.00000000

<p>Li₇Al-IV ($D_{5h}, ^1A_1'$)</p>	<p>Li 1.56484010 2.15381763 -0.00000000 Li -1.56484010 2.15381763 -0.00000000 Al 0.00000000 -0.00000000 0.00000000</p>
 <p>Li₇Al-V ($C_{3v}, ^1A_1$)</p>	<p>Li 0.00000000 1.75383562 -1.80796591 Li -2.18606879 1.26212741 0.69572833 Li -0.00000000 -0.00000000 2.79002097 Li 1.51886620 -0.87691781 -1.80796591 Li 0.00000000 -2.52425481 0.69572833 Li 2.18606879 1.26212741 0.69572833 Li -1.51886620 -0.87691781 -1.80796591 Al 0.00000000 -0.00000000 0.12615997</p>
 <p>Li₇Al-VI ($C_{2v}, ^1A_1$)</p>	<p>Li -0.11206300 1.78423600 1.54666200 Li -0.11206300 -1.78423600 1.54666300 Li 2.22856600 -3.03897700 0.00000000 Li -0.11206300 1.78423600 -1.54666200 Li 2.22854500 3.03898000 0.00000000 Li 1.46869600 0.00000300 0.00000000 Al -1.26405100 -0.00000200 0.00000000 Li -0.11206300 -1.78423600 -1.54666300</p>
 <p>Li₇Al-IIIc ($C_{3v}, ^2A_1$)</p>	<p>Li 1.51886600 0.87691800 -1.80796600 Li 0.00000000 2.52425500 0.69572800 Li 0.00000000 0.00000000 2.79002100 Li 0.00000000 -1.75383600 -1.80796600 Li -2.18606900 -1.26212700 0.69572800 Li 2.18606900 -1.26212700 0.69572800 Li -1.51886600 0.87691800 -1.80796600 Al 0.00000000 0.00000000 0.12616000</p>
 <p>Li₇Al-IIIc ($C_{2v}, ^2A_1$)</p>	<p>Li 0.00000000 0.00000000 -2.47183515 Li 1.67924836 -1.87178534 -0.52878696 Li -1.67924836 -1.87178534 -0.52878696 Li 1.67924836 1.87178534 -0.52878696 Li -1.67924836 1.87178534 -0.52878696 Li 0.00000000 1.79453878 2.03496805 Li 0.00000000 -1.79453878 2.03496805 Al 0.00000000 0.00000000 0.11928785</p>
 <p>Li₇Al-IV ($D_{5h}, ^2A_1'$)</p>	<p>Li 0.00000000 -2.61089560 0.00000000 Li 0.00000000 0.00000000 -2.54151191 Li -2.48310928 -0.80681111 0.00000000 Li 0.00000000 0.00000000 2.54151191 Li 2.48310928 -0.80681111 0.00000000 Li 1.53464593 2.11225891 0.00000000 Li -1.53464593 2.11225891 0.00000000 Al 0.00000000 0.00000000 0.00000000</p>

 Li₈Al-II ($C_{s, 2A'}$)	Li -1.86357005 0.86507335 -1.39018421 Li 1.85804209 -2.23929913 -0.29527621 Li -4.21443301 -0.48322730 0.16156316 Li -1.56065008 0.72126318 1.30644584 Li 0.56859384 2.48551999 0.30946734 Li 1.31208996 -0.36376247 1.98795421 Li 3.11002296 0.44233191 -0.35460800 Al 0.51234998 0.06034977 -0.41238893 Li -1.43027894 -1.68941519 0.06165657
 Li₈Al-I ($C_{2v, 2A_1}$)	Li 0.00000000 -2.23713601 1.17031330 Li 1.95152718 1.61208556 -1.07422415 Li -1.95152718 -1.61208556 -1.07422415 Li -1.95152718 1.61208556 -1.07422415 Li -2.12108405 0.00000000 1.37241623 Li 2.12108405 0.00000000 1.37241623 Li 1.95152718 -1.61208556 -1.07422415 Li -0.00000000 2.23713601 1.17031330 Al 0.00000000 0.00000000 -0.18203189
 Li₈Al-Ic ($C_{3v, 1A_1}$)	Li 1.38107700 0.79736500 -1.56870900 Li 0.00000000 -1.59473000 -1.56870900 Li -1.38107700 0.79736500 -1.56870900 Li 0.00000000 2.50496900 1.09964600 Li 2.16936700 -1.25248500 1.09964600 Li 0.00000000 0.00000000 -4.26194700 Li -2.16936700 -1.25248500 1.09964600 Li 0.00000000 0.00000000 3.22033100 Al 0.00000000 0.00000000 0.56510800
 Li₈Al-IIc ($D_{2d, 1A_1}$)	Li -1.03475600 1.69535900 1.69539900 Li -1.03475600 -1.69535900 -1.69539900 Li 1.03475600 1.69535900 -1.69539900 Li 2.33926200 -1.01868400 -1.01865900 Li 2.33926200 1.01868400 1.01865900 Li -2.33926200 -1.01868400 1.01865900 Li -2.33926200 1.01868400 -1.01865900 Li 1.03475600 -1.69535900 1.69539900 Al -0.00000000 0.00000000 0.00000000