

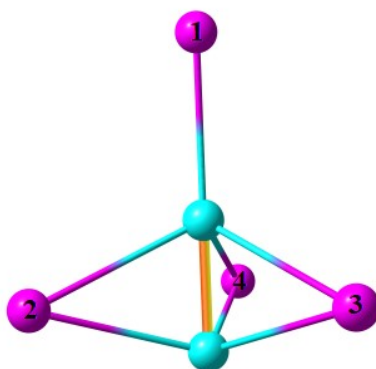
Ultra High Reversible Hydrogen Storage Capacity of Li_4B_2 Cluster: A Quantum Chemical Study

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TableS1: The charge transfer calculated on the four Li atom separately after the adsorption of H_2 using $\omega\text{B97XD/def2TZVP}$ level.



Complex	Charge Transfer(e)			
	Li (1)	Li (2)	Li(3)	Li(4)
Li_4B_2	0.789	0.759	0.759	0.759
$\text{Li}_4\text{B}_2\text{-1H}_2$	0.004			
$\text{Li}_4\text{B}_2\text{-2H}_2$	0.010			
$\text{Li}_4\text{B}_2\text{-3H}_2$	0.021			
$\text{Li}_4\text{B}_2\text{-4H}_2$	0.033			
$\text{Li}_4\text{B}_2\text{-5H}_2$		0.013		
$\text{Li}_4\text{B}_2\text{-6H}_2$			0.015	
$\text{Li}_4\text{B}_2\text{-7H}_2$				0.030
$\text{Li}_4\text{B}_2\text{-8H}_2$		0.038		
$\text{Li}_4\text{B}_2\text{-9H}_2$			0.040	
$\text{Li}_4\text{B}_2\text{-10H}_2$				0.042
$\text{Li}_4\text{B}_2\text{-11H}_2$		0.024		
$\text{Li}_4\text{B}_2\text{-12H}_2$			0.015	
$\text{Li}_4\text{B}_2\text{-13H}_2$				0.018

Cartesian coordinates of the low-lying isomers at ω B97XD/def2-TZVP level.

Li₄B₂

5	1.097605000	0.000466000	-0.002410000
5	-0.424632000	-0.000125000	0.000803000
3	0.470774000	-1.466600000	-1.388158000
3	0.472841000	1.936315000	-0.574440000
3	-2.543309000	0.000412000	0.003124000
3	0.478071000	-0.470695000	1.962152000

Li₄B₂-1H₂

5	1.497439156	-0.010109692	-0.003917782
5	-0.025646352	0.003843580	0.001279556
3	0.866676915	-1.152224255	1.656372812
3	0.858198855	-0.858087400	-1.828777040
3	-2.139606067	0.021169685	0.006010224
3	0.890635516	2.004556535	0.171626584
1	-4.399227957	0.365183324	-0.021301356
1	-4.387451715	-0.380096447	0.018794746

Li₄B₂-2H₂

5	-1.731424000	0.002500000	0.066959000
5	-0.211019000	-0.001597000	-0.032773000
3	-1.180678000	-1.770729000	-0.930316000
3	-0.979905000	0.064274000	2.035327000
3	1.898505000	-0.007833000	-0.169389000
3	-1.180044000	1.704253000	-1.047125000
1	3.237941000	-1.739923000	0.110201000
1	3.806685000	-1.275288000	-0.032867000
1	3.786901000	1.295451000	-0.029898000

1	3.207055000	1.745356000	0.116142000
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Li₄B₂-3H₂

5	1.916570000	-0.001781000	-0.000309000
5	0.392978000	0.001677000	-0.000324000
3	1.306199000	0.795383000	-1.849842000
3	1.307519000	1.203423000	1.613953000
3	-1.724496000	0.005198000	-0.001714000
3	1.299723000	-2.000379000	0.235375000
1	-2.697218000	1.905617000	-0.205331000
1	-3.352754000	1.542825000	-0.165182000
1	-3.348591000	-0.918638000	-1.251525000
1	-2.682861000	-0.774876000	1.750385000
1	-3.342191000	-0.630269000	1.422514000
1	-2.690959000	-1.135010000	-1.541012000

Li₄B₂-4H₂

5	-1.996096000	-0.006994000	0.027959000
5	-0.473162000	-0.002833000	0.009729000
3	-1.402743000	1.613080000	1.216867000
3	-1.444017000	0.215877000	-1.979333000
3	1.661025000	0.001282000	-0.017496000
3	-1.402766000	-1.856928000	0.810577000
1	2.099179000	1.451983000	-1.481402000
1	2.901117000	-1.300495000	1.330213000
1	2.937086000	1.345071000	1.271206000
1	2.083963000	-1.480523000	-1.452468000
1	2.821956000	-1.362978000	-1.355429000
1	2.207485000	1.467248000	1.409404000
1	2.168167000	-1.405174000	1.467677000
1	2.836014000	1.326579000	-1.387314000

Li₄B₂-5H₂

5	1.678693000	-0.869644000	0.010769000
5	0.242740000	-0.361460000	0.004294000
3	0.771497000	-1.654693000	1.725859000
3	0.795559000	-1.648645000	-1.717504000
3	-1.773709000	0.335963000	-0.008940000
3	1.827854000	1.217309000	0.000404000
1	-2.849910000	-1.422536000	-0.378638000
1	-2.290316000	2.495975000	0.333126000
1	-3.060081000	0.425525000	1.820305000
1	-2.022177000	0.874798000	-2.014054000
1	-2.737701000	1.069177000	-1.876850000
1	-2.369287000	0.187321000	2.003065000
1	-1.548060000	2.384606000	0.396078000
1	-3.493158000	-1.029349000	-0.374776000
1	2.631747000	3.404811000	0.005103000
1	3.268182000	3.015388000	0.011869000

Li₄B₂-6H₂

5	-1.698369000	0.127543000	0.590752000
5	-0.209973000	0.006363000	0.290261000
3	-0.725254000	0.042565000	2.439732000
3	-1.211351000	1.858595000	-0.466855000
3	1.876369000	-0.149608000	-0.123691000
3	-1.488544000	-1.643154000	-0.499054000
1	2.545772000	1.730682000	0.478515000
1	2.805612000	-1.985357000	-1.007438000
1	3.398102000	-0.878330000	1.336590000
1	1.921168000	0.502045000	-2.103668000

1	2.672831000	0.438021000	-2.118795000
1	2.710308000	-0.924295000	1.640623000
1	2.069706000	-2.092092000	-0.886444000
1	3.246244000	1.559067000	0.256810000
1	-0.997698000	3.875051000	-1.602285000
1	-1.723118000	3.902036000	-1.430073000
1	-1.884555000	-3.655776000	-1.612191000
1	-2.576321000	-3.465778000	-1.407109000

Li₄B₂-7H₂

5	-1.651558000	-0.119566000	0.342518000
5	-0.159630000	-0.049209000	0.042355000
3	-0.737557000	-1.323585000	1.778440000
3	-1.141743000	1.892967000	0.529501000
3	1.929029000	0.055357000	-0.373644000
3	-1.438902000	-0.810140000	-1.614613000
1	2.613497000	1.227092000	1.198644000
1	2.817296000	-1.023088000	-2.122874000
1	3.336148000	-1.456359000	0.491098000
1	2.008292000	1.698636000	-1.635004000
1	2.755903000	1.618094000	-1.702293000
1	2.617407000	-1.608297000	0.663040000
1	2.078754000	-1.160856000	-2.054194000
1	3.313079000	1.185853000	0.918384000
1	-1.079566000	4.213563000	0.823037000
1	-1.805612000	4.084914000	0.936760000
1	-1.979596000	-1.662632000	-3.737042000
1	-2.649410000	-1.573163000	-3.420627000
1	-0.235310000	-2.588422000	3.670525000
1	-0.234200000	-3.121218000	3.148151000

Li₄B₂-8H₂

5	-1.475904000	-0.709659000	0.156934000
5	-0.053802000	-0.180448000	0.012288000
3	-0.435023000	-1.453385000	1.799492000
3	-1.661993000	1.370548000	0.111496000
3	1.936135000	0.558540000	-0.187247000
3	-0.750886000	-1.528223000	-1.615616000
1	1.849354000	2.109417000	1.171868000
1	3.436101000	-0.333793000	-1.559909000
1	3.616568000	-0.132890000	1.094341000
1	1.639733000	1.902210000	-1.721924000
1	2.360186000	2.127847000	-1.684108000
1	2.985172000	-0.511133000	1.258572000
1	2.797361000	-0.734537000	-1.572610000
1	2.552127000	2.325000000	0.996100000
1	-3.687641000	2.499360000	0.255068000
1	-3.802634000	1.758364000	0.288200000
1	-0.486557000	-2.680708000	-3.639378000
1	-1.184194000	-2.870795000	-3.455751000
1	0.339560000	-2.105586000	3.892517000
1	0.103135000	-2.769129000	3.646869000
1	-1.403765000	3.671038000	-0.030175000
1	-0.730675000	3.353424000	-0.110165000

Li₄B₂-9H₂

5	-1.463663000	-0.007383000	0.584642000
5	0.003266000	-0.016352000	0.168239000
3	-0.380299000	0.063275000	2.357256000

3	-1.206025000	1.705326000	-0.579050000
3	2.055764000	-0.024977000	-0.410597000
3	-1.187546000	-1.808167000	-0.431415000
1	2.401204000	2.002299000	-0.516316000
1	3.112577000	-1.945870000	-0.661199000
1	3.718504000	0.035878000	1.058317000
1	1.801864000	-0.093626000	-2.437069000
1	2.551179000	-0.091955000	-2.544330000
1	3.050218000	0.051748000	1.408048000
1	2.421380000	-2.047864000	-0.372888000
1	3.095560000	1.889687000	-0.792564000
1	-2.896509000	-3.298369000	-0.956351000
1	-3.182015000	2.634072000	-0.643166000
1	0.017548000	-2.974308000	-1.863171000
1	-0.507649000	-3.507848000	-1.867953000
1	0.392844000	0.589322000	4.483547000
1	0.273415000	-0.139620000	4.588344000
1	-0.573144000	3.355062000	-2.088718000
1	-0.038991000	2.830863000	-2.077739000
1	-2.943054000	3.171023000	-1.110317000
1	-3.177746000	-2.697487000	-0.605307000

Li₄B₂-10H₂

5	-1.637208000	-0.771672000	0.119949000
5	-0.189090000	-0.310657000	-0.017523000
3	-0.629698000	-1.587937000	1.753263000
3	-1.713660000	1.307884000	0.176874000
3	1.836191000	0.326315000	-0.216192000
3	-0.998626000	-1.505342000	-1.720574000
1	1.845844000	1.854643000	1.149723000

1	3.201248000	-0.698092000	-1.617988000
1	3.449610000	-0.507217000	1.052451000
1	1.582003000	1.665567000	-1.737299000
1	2.317784000	1.843688000	-1.723706000
1	2.786901000	-0.840088000	1.194582000
1	2.529923000	-1.043298000	-1.584323000
1	2.560240000	2.028915000	0.971905000
1	-2.389171000	-2.658828000	-3.199969000
1	-3.823453000	1.840603000	0.400372000
1	0.335414000	-1.270547000	-3.457501000
1	-0.048018000	-1.801531000	-3.820181000
1	0.956708000	-1.482290000	3.288280000
1	0.618786000	-2.042990000	3.650867000
1	-1.313131000	3.599386000	0.132488000
1	-0.665279000	3.238536000	0.029337000
1	-3.662313000	2.573710000	0.400652000
1	-2.761987000	-2.469174000	-2.576397000
1	-1.779912000	-2.854688000	3.354823000
1	-2.237973000	-2.618452000	2.808038000

Li₄B₂-11H₂

5	-1.617641000	-0.763918000	0.089853000
5	-0.185761000	-0.251978000	-0.023819000
3	-0.650296000	-1.448856000	1.800840000
3	-1.767072000	1.312752000	0.123110000
3	1.821132000	0.444903000	-0.205841000
3	-0.897174000	-1.551224000	-1.706401000
1	1.915470000	1.565024000	1.490302000
1	2.994817000	-0.204254000	-1.964239000
1	3.448989000	-0.745432000	0.648752000

1	1.475353000	2.116109000	-1.318348000
1	2.210141000	2.298027000	-1.304674000
1	2.780088000	-1.089845000	0.731762000
1	2.295694000	-0.492221000	-1.960326000
1	2.631485000	1.758691000	1.336815000
1	-0.283304000	-0.448715000	-3.484315000
1	-3.895864000	1.764386000	0.321167000
1	0.654313000	-3.055483000	-2.009263000
1	0.376917000	-3.226009000	-2.684846000
1	1.074876000	-1.266716000	3.153913000
1	0.765295000	-1.758436000	3.626356000
1	-1.440446000	3.612892000	0.286198000
1	-0.774919000	3.270416000	0.307213000
1	-3.765149000	2.503619000	0.317247000
1	-0.393305000	-1.045748000	-3.925397000
1	-1.636540000	-2.678773000	3.517333000
1	-2.139477000	-2.529282000	2.980627000
1	-2.282293000	-2.777876000	-3.011212000
1	-2.640998000	-2.549582000	-2.389152000

Li₄B₂-12H₂

5	-1.693996000	-0.646150000	0.117448000
5	-0.251943000	-0.161256000	0.031832000
3	-0.770329000	-1.353901000	1.842745000
3	-1.825116000	1.436844000	0.114878000
3	1.759181000	0.531311000	-0.120849000
3	-0.920381000	-1.545720000	-1.600228000
1	1.949576000	1.243786000	1.762825000
1	2.759432000	0.300457000	-2.064285000
1	3.369824000	-0.858576000	0.320762000

1	1.334541000	2.405390000	-0.768482000
1	2.066002000	2.601129000	-0.772806000
1	2.690762000	-1.187692000	0.393175000
1	2.040225000	0.064533000	-2.078706000
1	2.664927000	1.455354000	1.627734000
1	-0.622746000	-0.503417000	-3.497649000
1	-3.867259000	1.730715000	0.614846000
1	0.888788000	-2.694628000	-1.876728000
1	0.639377000	-2.994640000	-2.518515000
1	1.065957000	-1.506805000	3.044503000
1	0.705049000	-1.904144000	3.566861000
1	-2.056383000	3.249260000	-1.337145000
1	-1.689959000	2.690789000	-1.677389000
1	-3.778035000	2.478058000	0.586483000
1	-0.641651000	-1.145315000	-3.884978000
1	-1.771521000	-2.596147000	3.544559000
1	-2.271284000	-2.440660000	3.006720000
1	-2.115786000	-3.094594000	-2.728396000
1	-2.504507000	-2.850775000	-2.131039000
1	-1.265464000	3.424497000	1.169599000
1	-0.761189000	2.884889000	1.307414000

Li₄B₂-13H₂

5	-1.473802000	-0.704574000	0.238590000
5	-0.067014000	-0.140133000	0.094130000
3	-0.441214000	-1.424494000	1.900226000
3	-1.730344000	1.364175000	0.251745000
3	1.903395000	0.654353000	-0.117660000
3	-0.743104000	-1.489813000	-1.556701000
1	1.915504000	1.574639000	1.662730000

1	3.029893000	0.274203000	-1.934104000
1	3.548713000	-0.564767000	0.616824000
1	1.320780000	2.374506000	-0.987749000
1	2.026331000	2.652558000	-0.996462000
1	2.879235000	-0.912556000	0.693517000
1	2.345172000	-0.047370000	-1.960585000
1	2.612118000	1.854601000	1.547744000
1	-0.389647000	-0.509880000	-3.479245000
1	-3.696922000	1.689236000	1.016799000
1	0.989114000	-2.774269000	-1.815064000
1	0.713088000	-3.078864000	-2.443492000
1	0.913792000	-0.397363000	3.217224000
1	0.879895000	-0.922803000	3.753927000
1	-2.110103000	3.138911000	-1.239109000
1	-1.779155000	2.558170000	-1.578813000
1	-3.595994000	2.430687000	0.939607000
1	-0.480616000	-1.164447000	-3.833189000
1	-1.482890000	-2.335974000	3.691607000
1	-1.991435000	-2.131755000	3.175455000
1	-2.001088000	-3.052726000	-2.611106000
1	-2.340127000	-2.805230000	-1.984426000
1	-1.051213000	3.383675000	1.202878000
1	-0.529167000	2.843487000	1.243058000
1	0.747608000	-3.312976000	2.599814000
1	0.841636000	-3.203713000	1.864257000

Cartesian coordinates of the low-lying isomers at B3LYP/def2-TZVP level

Li₄B₂

5	1.482700000	-0.009595000	-0.003055000
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5	-0.038379000	0.001638000	-0.000201000
3	0.816501000	-1.137106000	1.637314000
3	0.812228000	-0.846774000	-1.807344000
3	-2.137389000	0.015210000	0.002883000
3	0.836729000	1.980100000	0.169300000

Li₄B₂-1H₂

5	1.480932000	-0.009758000	-0.003146000
5	-0.041486000	0.001747000	-0.000150000
3	0.815699000	-1.135982000	1.636432000
3	0.811456000	-0.846006000	-1.806380000
3	-2.130138000	0.015095000	0.002855000
3	0.835927000	1.978378000	0.169287000
1	-4.310266000	0.368312000	-0.017817000
1	-4.301104000	-0.377549000	0.019008000

Li₄B₂-2H₂

5	-1.686142000	-0.001412000	0.049057000
5	-0.164582000	-0.001288000	-0.010142000
3	-1.075528000	-1.762682000	-0.900859000
3	-0.961074000	0.075969000	2.009684000
3	1.927379000	-0.000377000	-0.084955000
3	-1.081607000	1.683579000	-1.033382000
1	3.127642000	-1.711414000	0.036337000
1	3.735582000	-1.278035000	-0.035147000
1	3.722532000	1.293357000	-0.011643000
1	3.109816000	1.718766000	0.067311000

Li₄B₂-3H₂

5	1.784699000	0.000871000	-0.002285000
5	0.262633000	-0.000179000	-0.000495000
3	1.155688000	0.793810000	-1.825077000

3	1.159005000	1.183388000	1.596995000
3	-1.849156000	-0.002571000	0.002512000
3	1.159294000	-1.975385000	0.223885000
1	-2.530709000	1.851859000	-0.204354000
1	-3.230911000	1.572264000	-0.173123000
1	-3.231051000	-0.940768000	-1.273533000
1	-2.532458000	-0.749587000	1.711892000
1	-3.232088000	-0.635733000	1.453197000
1	-2.531026000	-1.104799000	-1.502627000

Li₄B₂-4H₂

5	-1.912266000	0.005612000	0.024427000
5	-0.391604000	0.023072000	-0.019382000
3	-1.299558000	1.703990000	1.052829000
3	-1.379053000	0.075934000	-1.980240000
3	1.751152000	0.049480000	-0.079296000
3	-1.268982000	-1.752897000	0.922464000
1	1.981879000	1.358338000	-1.583464000
1	2.881390000	-1.148014000	1.313508000
1	2.883167000	1.473230000	1.087900000
1	1.997775000	-1.465497000	-1.359112000
1	2.747813000	-1.369925000	-1.321052000
1	2.142007000	1.560968000	1.207178000
1	2.139696000	-1.213452000	1.445453000
1	2.732780000	1.276621000	-1.538138000

Li₄B₂-5H₂

5	1.627405000	-0.882768000	0.355129000
5	0.202005000	-0.362320000	0.243716000
3	0.754218000	-1.102011000	2.225304000
3	0.654984000	-2.079765000	-1.033140000
3	-1.810768000	0.364834000	0.092220000
3	1.811485000	1.086125000	-0.252789000

1	-2.700189000	-1.237713000	-0.731658000
1	-2.189996000	2.341571000	0.793390000
1	-3.220311000	0.086069000	1.688590000
1	-1.621265000	1.148184000	-1.719147000
1	-2.336293000	1.397390000	-1.684277000
1	-2.557805000	-0.234051000	1.863885000
1	-1.469375000	2.143257000	0.917623000
1	-3.354607000	-0.858672000	-0.754164000
1	2.536960000	2.999180000	-1.254069000
1	2.595995000	3.205295000	-0.539187000

Li₄B₂-6H₂

5	-1.672715000	0.105319000	0.614361000
5	-0.191512000	-0.013754000	0.286170000
3	-0.664845000	-0.158476000	2.407863000
3	-1.162593000	1.893744000	-0.286629000
3	1.901490000	-0.190737000	-0.163089000
3	-1.508787000	-1.550300000	-0.612271000
1	2.357946000	1.730592000	0.023124000
1	2.673093000	-2.125423000	-0.582838000
1	3.355109000	-0.510683000	1.370545000
1	1.688735000	0.035441000	-2.104834000
1	2.439908000	-0.034418000	-2.189588000
1	2.662878000	-0.468914000	1.674069000
1	1.940431000	-2.161329000	-0.392308000
1	3.070696000	1.581570000	-0.187050000
1	-1.207913000	3.816797000	-1.538322000
1	-1.146096000	4.116571000	-0.857726000
1	-1.909701000	-3.203842000	-2.154339000
1	-1.895197000	-3.614580000	-1.531460000

Li₄B₂-7H₂

5	-1.652698000	-0.131133000	0.393615000
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5	-0.168881000	-0.057327000	0.061993000
3	-0.723467000	-1.454752000	1.677400000
3	-1.108117000	1.832046000	0.719853000
3	1.923881000	0.048065000	-0.420060000
3	-1.504618000	-0.681971000	-1.588137000
1	2.380059000	1.552310000	0.769345000
1	2.673261000	-1.349084000	-1.803943000
1	3.294782000	-1.081324000	0.733048000
1	1.716083000	1.294788000	-1.925378000
1	2.467334000	1.274439000	-2.034542000
1	2.585091000	-1.178210000	0.981990000
1	1.936810000	-1.473061000	-1.668165000
1	3.094952000	1.528782000	0.516541000
1	-1.156779000	4.143536000	0.796821000
1	-1.066596000	4.005335000	1.524540000
1	-1.920113000	-1.028935000	-3.844545000
1	-1.872425000	-1.737728000	-3.616368000
1	-0.239592000	-2.739772000	3.556214000
1	-0.302647000	-3.286063000	3.051940000

Li₄B₂-8H₂

5	-1.448714000	-0.622927000	0.181393000
5	-0.021616000	-0.118592000	0.015079000
3	-0.433116000	-1.284404000	1.847762000
3	-1.613556000	1.438515000	0.060843000
3	2.008945000	0.555540000	-0.221020000
3	-0.732056000	-1.521722000	-1.531085000
1	1.941986000	1.827171000	1.253054000
1	3.221590000	-0.285436000	-1.741274000
1	3.531661000	-0.441821000	0.853043000
1	1.592873000	1.964852000	-1.511495000
1	2.325179000	2.167888000	-1.519947000
1	2.858805000	-0.771495000	0.971280000

1	2.535647000	-0.608112000	-1.736764000
1	2.659521000	2.027379000	1.100618000
1	-3.735677000	2.419201000	0.210837000
1	-3.726213000	1.668129000	0.260269000
1	-0.609012000	-2.438948000	-3.682704000
1	-0.430639000	-3.045399000	-3.286428000
1	0.158825000	-1.857601000	4.032830000
1	0.211174000	-2.531358000	3.716646000
1	-1.525777000	3.696510000	-0.068391000
1	-0.827473000	3.428091000	-0.097682000

Li₄B₂-9H₂

5	-1.400422000	0.013527000	0.487701000
5	0.068634000	0.006716000	0.085222000
3	-0.341420000	0.061983000	2.252771000
3	-1.138125000	1.723773000	-0.649493000
3	2.160723000	-0.011463000	-0.425874000
3	-1.129298000	-1.747680000	-0.567390000
1	2.372085000	1.927552000	-0.633564000
1	3.123990000	-1.873155000	-0.459172000
1	3.602887000	0.159194000	1.115631000
1	1.877559000	-0.198611000	-2.341583000
1	2.631514000	-0.206103000	-2.442780000
1	2.900292000	0.184883000	1.400014000
1	2.400567000	-1.946204000	-0.238689000
1	3.096385000	1.823429000	-0.836138000
1	-2.933861000	-3.236898000	-0.852944000
1	-3.100475000	2.603881000	-0.536671000
1	-0.047634000	-3.016563000	-1.936943000
1	-0.610057000	-3.510590000	-1.924080000
1	0.321431000	0.412016000	4.494464000
1	0.354607000	-0.332856000	4.469673000
1	-0.684133000	3.379146000	-2.160764000

1	-0.139744000	2.866051000	-2.189728000
1	-2.958917000	3.208238000	-0.961952000
1	-3.087907000	-2.615537000	-0.457465000

Li₄B₂-10H₂

5	-1.548270000	-0.693374000	0.099529000
5	-0.098949000	-0.243013000	-0.035478000
3	-0.579259000	-1.481279000	1.746269000
3	-1.619469000	1.372303000	0.130476000
3	1.958229000	0.378584000	-0.222998000
3	-0.918075000	-1.442181000	-1.720557000
1	1.872291000	1.715114000	1.187570000
1	3.172171000	-0.583799000	-1.647476000
1	3.411790000	-0.596177000	0.943802000
1	1.617670000	1.725748000	-1.583653000
1	2.357543000	1.903021000	-1.578505000
1	2.724279000	-0.898162000	1.056416000
1	2.475966000	-0.886322000	-1.633864000
1	2.598410000	1.894252000	1.047922000
1	-2.441299000	-2.760934000	-3.005944000
1	-3.729854000	1.732531000	0.339057000
1	0.273294000	-1.383597000	-3.537259000
1	-0.157077000	-1.920181000	-3.832385000
1	0.924035000	-1.517085000	3.324777000
1	0.537248000	-2.056435000	3.670379000
1	-1.422678000	3.651651000	0.112399000
1	-0.744322000	3.346438000	0.028001000
1	-3.702633000	2.484600000	0.344472000
1	-2.695246000	-2.501458000	-2.346633000
1	-1.866719000	-2.852768000	3.261380000
1	-2.227941000	-2.571033000	2.664252000

Li₄B₂-11H₂

5	-1.533253000	-0.681218000	0.043883000
5	-0.094820000	-0.194590000	-0.070298000
3	-0.598571000	-1.349378000	1.761714000
3	-1.646211000	1.384898000	0.063543000
3	1.941719000	0.492355000	-0.229584000
3	-0.822443000	-1.540596000	-1.716824000
1	2.004669000	1.362525000	1.512896000
1	2.998650000	0.031024000	-2.002667000
1	3.435825000	-0.805149000	0.435871000
1	1.568452000	2.213104000	-1.093884000
1	2.310884000	2.373258000	-1.081765000
1	2.748431000	-1.122805000	0.507363000
1	2.284717000	-0.224564000	-2.028186000
1	2.728755000	1.551894000	1.377563000
1	-0.407693000	-0.565222000	-3.620848000
1	-3.806326000	1.644793000	0.296294000
1	0.679051000	-3.080665000	-1.870329000
1	0.421439000	-3.335076000	-2.527790000
1	1.044225000	-1.461554000	3.188916000
1	0.633053000	-1.895839000	3.638968000
1	-1.637157000	3.679885000	0.219120000
1	-0.929669000	3.437218000	0.240087000
1	-3.842134000	2.396511000	0.296970000
1	-0.526086000	-1.194768000	-4.010809000
1	-1.820175000	-2.620076000	3.397170000
1	-2.205063000	-2.395387000	2.791200000
1	-2.302385000	-2.829124000	-2.707250000
1	-2.553555000	-2.508982000	-2.067670000
Li₄B₂-12H₂			
5	-1.588632000	-0.609038000	0.133975000
5	-0.151844000	-0.120768000	0.017277000
3	-0.629772000	-1.328943000	1.818469000

3	-1.730183000	1.469239000	0.106911000
3	1.879321000	0.586397000	-0.132419000
3	-0.865609000	-1.517423000	-1.594272000
1	1.990089000	1.263137000	1.690175000
1	2.871929000	0.355868000	-1.973604000
1	3.400507000	-0.751990000	0.335895000
1	1.437043000	2.392084000	-0.756588000
1	2.174002000	2.574797000	-0.761866000
1	2.719046000	-1.083563000	0.402855000
1	2.158751000	0.098618000	-2.011921000
1	2.707701000	1.477125000	1.555653000
1	-0.831228000	-0.515621000	-3.600005000
1	-3.734653000	1.450141000	0.351384000
1	0.760822000	-2.850338000	-1.937503000
1	0.439657000	-3.128970000	-2.556128000
1	1.068501000	-1.559844000	3.149834000
1	0.657719000	-1.977579000	3.616022000
1	-1.956323000	3.276834000	-1.384223000
1	-1.529500000	2.725689000	-1.661253000
1	-3.797390000	2.205420000	0.340937000
1	-0.874019000	-1.150479000	-3.995687000
1	-1.827104000	-2.602546000	3.440539000
1	-2.222588000	-2.364401000	2.846256000
1	-2.275612000	-2.992727000	-2.489636000
1	-2.530081000	-2.659058000	-1.859106000
1	-1.554550000	3.428501000	1.349687000
1	-1.039907000	2.922030000	1.553531000

Li₄B₂-13H₂

5	-1.433340000	-0.677072000	0.270409000
5	-0.031948000	-0.111762000	0.097540000
3	-0.407834000	-1.343736000	1.948813000

3	-1.686247000	1.393762000	0.209118000
3	1.953769000	0.694136000	-0.154670000
3	-0.737319000	-1.544564000	-1.488131000
1	2.074730000	1.427409000	1.628423000
1	2.880345000	0.446744000	-2.021600000
1	3.511493000	-0.589481000	0.311571000
1	1.398414000	2.451126000	-0.808082000
1	2.125494000	2.667010000	-0.849969000
1	2.837812000	-0.932512000	0.401731000
1	2.177061000	0.160405000	-2.024764000
1	2.782205000	1.662424000	1.473007000
1	-0.820317000	-0.602252000	-3.506115000
1	-3.659188000	1.239620000	0.552040000
1	0.955352000	-2.787989000	-1.822030000
1	0.655844000	-3.103268000	-2.434369000
1	0.872459000	-0.455281000	3.366892000
1	0.738141000	-0.999155000	3.867484000
1	-2.063690000	3.165663000	-1.252955000
1	-1.608704000	2.647556000	-1.548671000
1	-3.774359000	1.989417000	0.536106000
1	-0.840093000	-1.254976000	-3.873513000
1	-1.717381000	-2.077784000	3.626930000
1	-2.090364000	-1.850117000	3.009205000
1	-2.071644000	-3.133277000	-2.301263000
1	-2.320118000	-2.810848000	-1.662497000
1	-1.597829000	3.364224000	1.470549000
1	-1.047355000	2.888370000	1.653659000
1	0.469848000	-3.532736000	2.743113000
1	0.426441000	-3.473530000	1.997960000