

Supporting Information

The structural effect of alkali-metals on B₁₂

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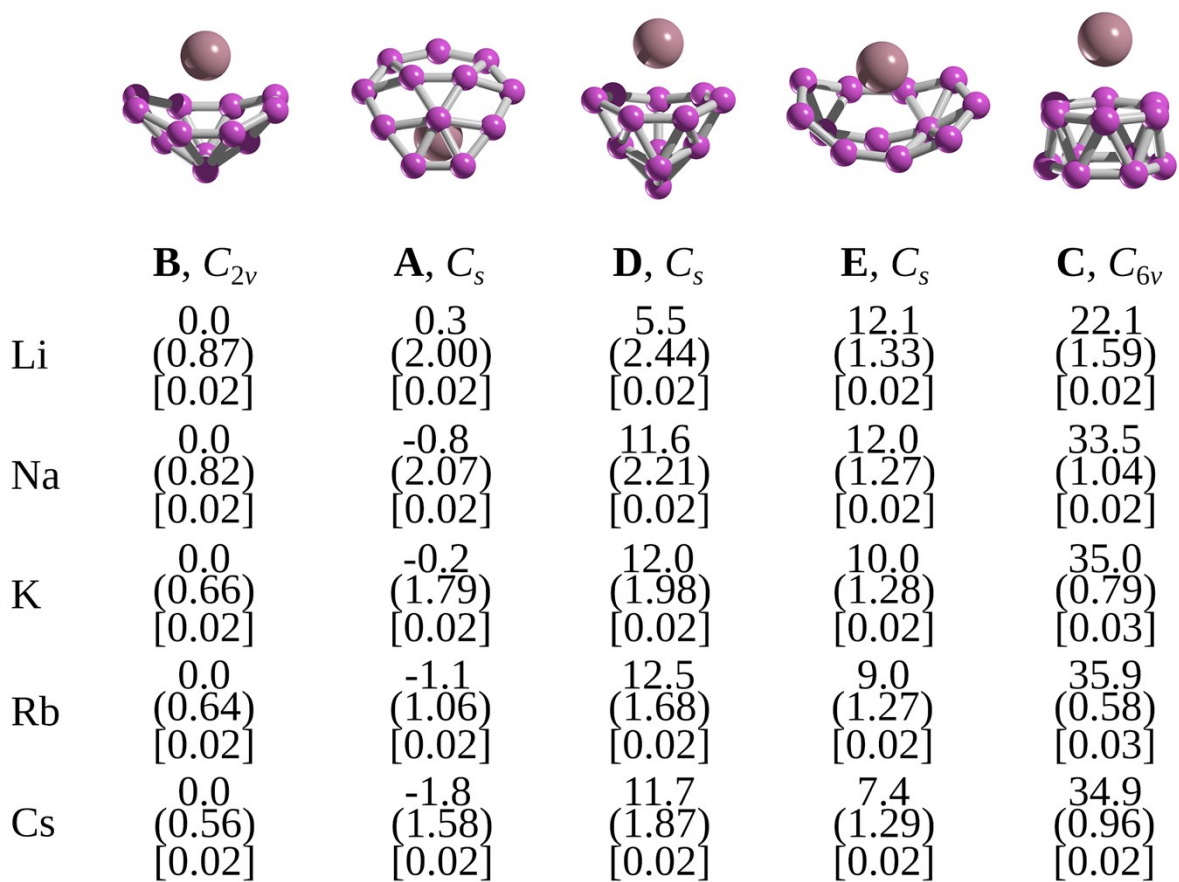


Figure S1. Relative energy, in kcal/mol, of the low-lying isomers of $B_{12}E^-$ ($E = \text{Li-Cs}$) clusters at the TPSS-D3/def2-TZVP level. The HOMO-LUMO energy difference, in eV, is between parentheses, and T1-diagnosis value between brackets.

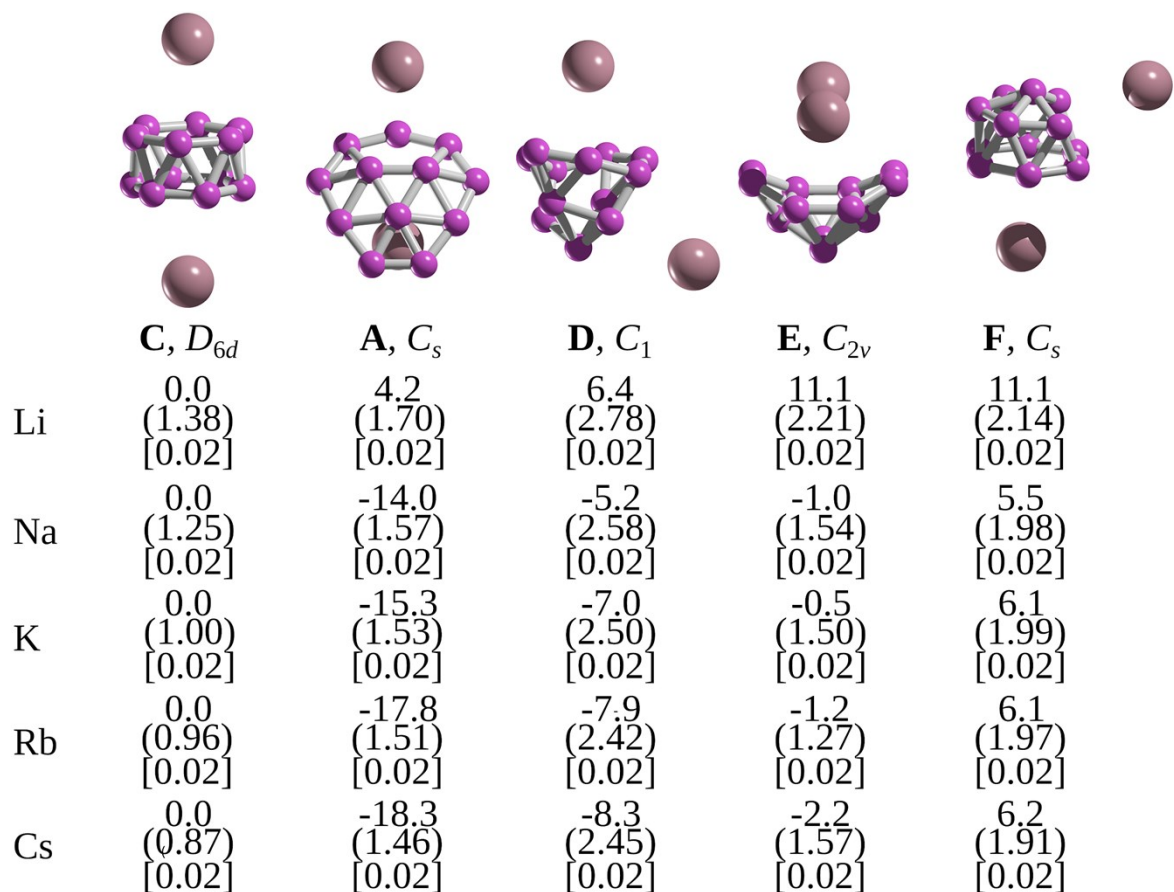


Figure S2. Relative energy, in kcal/mol, of the low-lying isomers of $B_{12}E_2$ ($E = \text{Li-Cs}$) clusters at the TPSS-D3/def2-TZVP level. The HOMO-LUMO energy difference, in eV, is between parentheses, and T1-diagnosis value between brackets.

Cartesian coordinates

13

A-Li

B	0.156837000	-1.807926000	1.502249000
B	-0.002665000	1.031812000	-1.705284000
B	0.231790000	2.353621000	0.772365000
B	0.072728000	-0.463555000	2.288817000
B	-0.002665000	1.031812000	1.705284000
B	0.231790000	2.353621000	-0.772365000
Li	1.442319000	-0.321071000	0.000000000
B	0.156837000	-1.807926000	-1.502249000
B	-0.755998000	-0.405031000	-0.826600000
B	0.155176000	-2.249930000	0.000000000
B	-0.425952000	1.024730000	-0.000000000
B	0.072728000	-0.463555000	-2.288817000
B	-0.755998000	-0.405031000	0.826600000

13

B-Li 0.0

B	0.805003000	1.626503000	0.079402000
B	-0.805003000	1.626503000	0.079402000
B	2.108358000	0.777777000	0.614906000
B	-2.108358000	0.777777000	0.614906000
Li	0.000000000	0.000000000	1.646882000
B	-0.805003000	-1.626503000	0.079402000
B	0.805003000	-1.626503000	0.079402000
B	-2.108358000	-0.777777000	0.614906000
B	0.000000000	-0.835809000	-1.289831000
B	1.264558000	-0.000000000	-0.592849000
B	0.000000000	0.835809000	-1.289831000
B	-1.264558000	0.000000000	-0.592849000
B	2.108358000	-0.777777000	0.614906000

13

D-Li

Li	-0.201375000	-1.992950000	-0.000000000
B	0.215215000	-0.887580000	1.917605000
B	1.391798000	-0.701118000	-0.827925000
B	-1.203837000	-0.488085000	-1.404092000
B	1.391798000	-0.701118000	0.827925000
B	-1.203837000	-0.488085000	1.404092000
B	0.215215000	-0.887580000	-1.917605000
B	-1.918376000	0.004026000	-0.000000000
B	0.365452000	1.904837000	0.000000000
B	0.215215000	0.603146000	1.127949000
B	0.215215000	0.603146000	-1.127949000

B	-1.108552000	1.413096000	-0.000000000
B	1.545520000	0.821085000	0.000000000
13			
E-Li			
B	0.756593000	1.734642000	0.000000000
B	0.267169000	1.092035000	1.464784000
B	0.442460000	-1.358910000	-0.000000000
B	0.267169000	-0.530227000	1.577492000
B	-0.468370000	2.429247000	0.797984000
B	0.267169000	1.092035000	-1.464784000
B	-0.437123000	-1.957299000	1.356889000
B	-0.437123000	-1.957299000	-1.356889000
Li	-1.340901000	0.173282000	0.000000000
B	-0.468370000	2.429247000	-0.797984000
B	-0.644790000	-2.695887000	-0.000000000
B	0.992589000	0.148676000	0.000000000
B	0.267169000	-0.530227000	-1.577492000
13			
C-Li			
B	0.800373000	1.386287000	-0.887523000
B	0.000000000	1.608830000	0.671936000
B	-1.393288000	0.804415000	0.671936000
B	-1.600746000	0.000000000	-0.887523000
B	-0.800373000	1.386287000	-0.887523000
B	1.600746000	-0.000000000	-0.887523000
B	1.393288000	-0.804415000	0.671936000
B	1.393288000	0.804415000	0.671936000
Li	0.000000000	0.000000000	2.155877000
B	-1.393288000	-0.804415000	0.671936000
B	-0.800373000	-1.386287000	-0.887523000
B	0.800373000	-1.386287000	-0.887523000
B	-0.000000000	-1.608830000	0.671936000
13			
A-Na			
B	-0.127322000	-1.780534000	1.511127000
B	-0.247892000	1.043229000	-1.710544000
B	0.074972000	2.345837000	0.772548000
B	-0.227969000	-0.444152000	2.310506000
B	-0.247892000	1.043229000	1.710544000
B	0.074972000	2.345837000	-0.772548000
Na	1.733302000	-0.207229000	0.000000000
B	-0.127322000	-1.780534000	-1.511127000
B	-1.002791000	-0.364506000	-0.828056000
B	-0.110573000	-2.195956000	0.000000000

B	-0.640688000	1.052110000	-0.000000000
B	-0.227969000	-0.444152000	-2.310506000
B	-1.002791000	-0.364506000	0.828056000

13

B-Na

B	0.807154000	1.621979000	-0.178626000
B	-0.807154000	1.621979000	-0.178626000
B	2.130945000	0.779124000	0.340249000
B	-2.130945000	0.779124000	0.340249000
Na	0.000000000	0.000000000	1.866845000
B	-0.807154000	-1.621979000	-0.178626000
B	0.807154000	-1.621979000	-0.178626000
B	-2.130945000	-0.779124000	0.340249000
B	-0.000000000	-0.837391000	-1.534999000
B	1.265381000	-0.000000000	-0.841776000
B	0.000000000	0.837391000	-1.534999000
B	-1.265381000	0.000000000	-0.841776000
B	2.130945000	-0.779124000	0.340249000

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D-Na

B	1.000724000	1.732712000	-0.000000000
B	0.510920000	1.070259000	1.452822000
B	0.650275000	-1.371487000	0.000000000
B	0.510920000	-0.550516000	1.573835000
B	-0.218850000	2.425547000	0.798971000
B	0.510920000	1.070259000	-1.452822000
B	-0.203953000	-1.975619000	1.362434000
B	-0.203953000	-1.975619000	-1.362434000
Na	-1.641804000	0.122010000	-0.000000000
B	-0.218850000	2.425547000	-0.798971000
B	-0.430365000	-2.705466000	0.000000000
B	1.193262000	0.136474000	-0.000000000
B	0.510920000	-0.550516000	-1.573835000

13

E-Na

Na	-0.233180000	-2.204237000	0.000000000
B	0.270983000	-0.554370000	1.938647000
B	1.433380000	-0.381391000	-0.824352000
B	-1.145778000	-0.184992000	-1.376820000
B	1.433380000	-0.381391000	0.824352000
B	-1.145778000	-0.184992000	1.376820000
B	0.270983000	-0.554370000	-1.938647000
B	-1.933966000	0.244925000	-0.000000000
B	0.339062000	2.201499000	-0.000000000

B	0.270983000	0.923438000	1.153918000
B	0.270983000	0.923438000	-1.153918000
B	-1.110089000	1.636459000	-0.000000000
B	1.558855000	1.161069000	0.000000000

13

C-Na

B	0.801043000	1.387447000	-1.218333000
B	0.000000000	1.608544000	0.342238000
B	-1.393040000	0.804272000	0.342238000
B	-1.602086000	0.000000000	-1.218333000
B	-0.801043000	1.387447000	-1.218333000
B	1.602086000	-0.000000000	-1.218333000
B	1.393040000	-0.804272000	0.342238000
B	1.393040000	0.804272000	0.342238000
Na	0.000000000	0.000000000	2.389349000
B	-1.393040000	-0.804272000	0.342238000
B	-0.801043000	-1.387447000	-1.218333000
B	0.801043000	-1.387447000	-1.218333000
B	-0.000000000	-1.608544000	0.342238000

13

A-K

B	-0.483951000	-1.780169000	1.509823000
B	-0.474629000	1.064927000	-1.704963000
B	-0.155260000	2.383441000	0.771743000
B	-0.480448000	-0.429357000	2.303069000
B	-0.474629000	1.064927000	1.704963000
B	-0.155260000	2.383441000	-0.771743000
K	1.854406000	-0.192954000	0.000000000
B	-0.483951000	-1.780169000	-1.509823000
B	-1.242814000	-0.315736000	-0.830256000
B	-0.511910000	-2.201121000	0.000000000
B	-0.860629000	1.088132000	-0.000000000
B	-0.480448000	-0.429357000	-2.303069000
B	-1.242814000	-0.315736000	0.830256000

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B-K

B	0.808234000	1.611478000	-0.466846000
B	-0.808234000	1.611478000	-0.466846000
B	2.149037000	0.778736000	0.027341000
B	-2.149037000	0.778736000	0.027341000
K	-0.000000000	-0.000000000	2.022222000
B	-0.808234000	-1.611478000	-0.466846000
B	0.808234000	-1.611478000	-0.466846000
B	-2.149037000	-0.778736000	0.027341000

B	0.000000000	-0.836888000	-1.827963000
B	1.269193000	-0.000000000	-1.135250000
B	0.000000000	0.836888000	-1.827963000
B	-1.269193000	0.000000000	-1.135250000
B	2.149037000	-0.778736000	0.027341000

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D-K

B	1.248480000	1.750491000	0.000000000
B	0.738416000	1.068480000	1.444422000
B	0.935653000	-1.404329000	0.000000000
B	0.738416000	-0.555780000	1.562531000
B	0.048815000	2.463226000	0.799301000
B	0.738416000	1.068480000	-1.444422000
B	0.113689000	-2.032145000	1.357448000
B	0.113689000	-2.032145000	-1.357448000
K	-1.777735000	0.108468000	0.000000000
B	0.048815000	2.463226000	-0.799301000
B	-0.048462000	-2.791333000	0.000000000
B	1.341048000	0.145434000	0.000000000
B	0.738416000	-0.555780000	-1.562531000

13

E-K

K	-2.299485000	-0.312364000	-0.000000000
B	-0.126046000	-0.356584000	1.952187000
B	0.297104000	-1.435014000	-0.822749000
B	-0.126046000	1.096109000	-1.355019000
B	0.297104000	-1.435014000	0.822749000
B	-0.126046000	1.096109000	1.355019000
B	-0.126046000	-0.356584000	-1.952187000
B	0.062548000	1.996225000	-0.000000000
B	2.535911000	0.264036000	0.000000000
B	1.305782000	-0.008624000	1.170098000
B	1.305782000	-0.008624000	-1.170098000
B	1.603892000	1.513553000	0.000000000
B	1.834104000	-1.178608000	0.000000000

13

C-K

B	0.800750000	1.386939000	-1.564803000
B	0.000000000	1.607579000	-0.002610000
B	-1.392205000	0.803790000	-0.002610000
B	-1.601500000	0.000000000	-1.564803000
B	-0.800750000	1.386939000	-1.564803000
B	1.601500000	-0.000000000	-1.564803000
B	1.392205000	-0.803790000	-0.002610000

B	1.392205000	0.803790000	-0.002610000
K	0.000000000	0.000000000	2.474863000
B	-1.392205000	-0.803790000	-0.002610000
B	-0.800750000	-1.386939000	-1.564803000
B	0.800750000	-1.386939000	-1.564803000
B	-0.000000000	-1.607579000	-0.002610000

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A-Rb

B	1.884266000	-0.574839000	1.511658000
B	-0.915522000	-1.090836000	-1.705791000
B	-2.273243000	-1.030714000	0.772202000
B	0.554456000	-0.820223000	2.305122000
B	-0.915522000	-1.090836000	1.705791000
B	-2.273243000	-1.030714000	-0.772202000
Rb	-0.148741000	1.647143000	0.000000000
B	1.884266000	-0.574839000	-1.511658000
B	0.583366000	-1.581191000	-0.830615000
B	2.300172000	-0.529407000	0.000000000
B	-0.866138000	-1.463845000	0.000000000
B	0.554456000	-0.820223000	-2.305122000
B	0.583366000	-1.581191000	0.830615000

13

B-Rb

B	0.808447000	1.610516000	-0.922689000
B	-0.808447000	1.610516000	-0.922689000
B	2.152422000	0.778911000	-0.433581000
B	-2.152422000	0.778911000	-0.433581000
Rb	-0.000000000	-0.000000000	1.781025000
B	-0.808447000	-1.610516000	-0.922689000
B	0.808447000	-1.610516000	-0.922689000
B	-2.152422000	-0.778911000	-0.433581000
B	0.000000000	-0.836970000	-2.284487000
B	1.269764000	-0.000000000	-1.592766000
B	0.000000000	0.836970000	-2.284487000
B	-1.269764000	0.000000000	-1.592766000
B	2.152422000	-0.778911000	-0.433581000

13

D-Rb

B	2.242402000	0.847709000	0.000000000
B	1.480449000	0.454832000	1.443009000
B	0.597569000	-1.869000000	0.000000000
B	0.777548000	-1.010952000	1.561237000
B	1.480449000	2.014592000	0.799699000
B	1.480449000	0.454832000	-1.443009000

B	-0.407683000	-2.093763000	1.357600000
B	-0.407683000	-2.093763000	-1.357600000
Rb	-1.384223000	0.762472000	0.000000000
B	1.480449000	2.014592000	-0.799699000
B	-0.869729000	-2.720303000	0.000000000
B	1.611477000	-0.630119000	0.000000000
B	0.777548000	-1.010952000	-1.561237000

13

E-Rb

Rb	-0.010599000	2.015018000	0.000000000
B	-0.336501000	-0.342444000	1.955754000
B	-1.458319000	-0.616872000	-0.822506000
B	1.101531000	-0.522311000	-1.347137000
B	-1.458319000	-0.616872000	0.822506000
B	1.101531000	-0.522311000	1.347137000
B	-0.336501000	-0.342444000	-1.955754000
B	1.981558000	-0.820292000	-0.000000000
B	-0.056543000	-3.054611000	-0.000000000
B	-0.179141000	-1.806682000	1.174911000
B	-0.179141000	-1.806682000	-1.174911000
B	1.298391000	-2.282548000	-0.000000000
B	-1.400116000	-2.177064000	-0.000000000

13

C-Rb

B	0.801121000	1.387582000	-2.100924000
B	0.000000000	1.607373000	-0.540004000
B	-1.392026000	0.803686000	-0.540004000
B	-1.602242000	0.000000000	-2.100924000
B	-0.801121000	1.387582000	-2.100924000
B	1.602242000	-0.000000000	-2.100924000
B	1.392026000	-0.803686000	-0.540004000
B	1.392026000	0.803686000	-0.540004000
Rb	0.000000000	0.000000000	2.141293000
B	-1.392026000	-0.803686000	-0.540004000
B	-0.801121000	-1.387582000	-2.100924000
B	0.801121000	-1.387582000	-2.100924000
B	-0.000000000	-1.607373000	-0.540004000

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A-Cs

B	1.873504000	-1.001618000	1.507177000
B	-0.964316000	-1.343409000	-1.702720000
B	-2.328577000	-1.243187000	0.771479000
B	0.520731000	-1.138043000	2.297552000
B	-0.964316000	-1.343409000	1.702720000

B	-2.328577000	-1.243187000	-0.771479000
Cs	-0.052361000	1.452387000	0.000000000
B	1.873504000	-1.001618000	-1.507177000
B	0.504244000	-1.902348000	-0.832582000
B	2.304380000	-0.999420000	0.000000000
B	-0.939579000	-1.719623000	0.000000000
B	0.520731000	-1.138043000	-2.297552000
B	0.504244000	-1.902348000	0.832582000

13

B-Cs

B	0.808605000	1.607368000	-1.270779000
B	-0.808605000	1.607368000	-1.270779000
B	2.154512000	0.778606000	-0.786785000
B	-2.154512000	0.778606000	-0.786785000
Cs	-0.000000000	-0.000000000	1.580837000
B	-0.808605000	-1.607368000	-1.270779000
B	0.808605000	-1.607368000	-1.270779000
B	-2.154512000	-0.778606000	-0.786785000
B	0.000000000	-0.836404000	-2.635690000
B	1.270580000	-0.000000000	-1.943786000
B	0.000000000	0.836404000	-2.635690000
B	-1.270580000	0.000000000	-1.943786000
B	2.154512000	-0.778606000	-0.786785000

13

D-Cs

B	1.862488000	-1.832360000	0.000000000
B	1.142364000	-1.349135000	1.442450000
B	-1.327813000	-1.761710000	0.000000000
B	-0.481700000	-1.456658000	1.557684000
B	2.515905000	-0.602541000	0.799054000
B	1.142364000	-1.349135000	-1.442450000
B	-2.024516000	-1.002049000	1.353702000
B	-2.024516000	-1.002049000	-1.353702000
Cs	-0.026608000	1.392733000	0.000000000
B	2.515905000	-0.602541000	-0.799054000
B	-2.807116000	-0.942955000	0.000000000
B	0.261028000	-1.962268000	0.000000000
B	-0.481700000	-1.456658000	-1.557684000

13

E-Cs

Cs	-0.006527000	1.764817000	0.000000000
B	-0.333371000	-0.719593000	1.958161000
B	-1.454224000	-0.984037000	-0.822975000
B	1.102623000	-0.902343000	-1.344989000

B	-1.454224000	-0.984037000	0.822975000
B	1.102623000	-0.902343000	1.344989000
B	-0.333371000	-0.719593000	-1.958161000
B	1.983631000	-1.201109000	-0.000000000
B	-0.065725000	-3.430457000	-0.000000000
B	-0.181454000	-2.182922000	1.174089000
B	-0.181454000	-2.182922000	-1.174089000
B	1.290953000	-2.659329000	-0.000000000
B	-1.404214000	-2.544304000	-0.000000000

13

E-Cs

B	0.799828000	1.385343000	-2.558812000
B	0.000000000	1.607195000	-0.995594000
B	-1.391872000	0.803598000	-0.995594000
B	-1.599656000	0.000000000	-2.558812000
B	-0.799828000	1.385343000	-2.558812000
B	1.599656000	0.000000000	-2.558812000
B	1.391872000	-0.803598000	-0.995594000
B	1.391872000	0.803598000	-0.995594000
Cs	0.000000000	0.000000000	1.779984000
B	-1.391872000	-0.803598000	-0.995594000
B	-0.799828000	-1.385343000	-2.558812000
B	0.799828000	-1.385343000	-2.558812000
B	0.000000000	-1.607195000	-0.995594000

14

C-Li

B	-0.000000000	1.607740000	0.767227000
B	1.392344000	0.803870000	0.767227000
B	-1.392344000	-0.803870000	0.767227000
B	-0.000000000	-1.607740000	0.767227000
Li	0.000000000	0.000000000	2.301840000
B	1.392344000	-0.803870000	0.767227000
B	-1.392344000	0.803870000	0.767227000
B	-0.803870000	1.392344000	-0.767227000
B	-0.803870000	-1.392344000	-0.767227000
Li	0.000000000	0.000000000	-2.301840000
B	-1.607740000	0.000000000	-0.767227000
B	0.803870000	1.392344000	-0.767227000
B	0.803870000	-1.392344000	-0.767227000
B	1.607740000	-0.000000000	-0.767227000

14

A-Li

B	0.052333000	1.128888000	1.720435000
B	-0.402129000	-1.646922000	1.478690000

B	0.709879000	-0.355453000	0.829946000
B	0.452553000	1.108511000	0.000000000
B	-0.152121000	2.435451000	0.774349000
B	-0.120679000	-0.356063000	2.303596000
B	-0.152121000	2.435451000	-0.774349000
Li	-1.646224000	-0.082331000	-0.000000000
B	-0.402129000	-1.646922000	-1.478690000
Li	1.595239000	-2.232982000	-0.000000000
B	0.709879000	-0.355453000	-0.829946000
B	-0.596530000	-2.131126000	-0.000000000
B	-0.120679000	-0.356063000	-2.303596000
B	0.052333000	1.128888000	-1.720435000

14

D-Li

B	-0.869528000	0.732782000	0.539547000
Li	-2.579886000	-0.638635000	0.588862000
B	-0.504984000	-0.436269000	1.702696000
B	-0.649537000	-1.490129000	0.487604000
B	-1.010748000	-1.064129000	-1.047878000
B	-1.457558000	0.503786000	-1.148773000
B	0.544427000	1.753522000	0.212172000
B	0.589381000	0.728500000	1.520647000
B	1.742576000	0.583228000	0.098647000
B	1.983938000	-0.795742000	-0.607265000
B	0.895735000	-0.800711000	0.703866000
B	0.590919000	-1.480566000	-0.894624000
B	-0.732172000	1.827684000	-0.766308000
Li	0.709140000	0.535375000	-1.922746000

14

E-Li

B	0.803444000	1.638074000	-0.126382000
B	-1.234744000	0.000000000	-0.654157000
B	1.985142000	0.773633000	0.615672000
B	-1.985142000	0.773633000	0.615672000
Li	0.000000000	1.539232000	1.861469000
B	-0.803444000	1.638074000	-0.126382000
B	0.000000000	0.817410000	-1.441304000
B	-1.985142000	-0.773633000	0.615672000
B	-0.000000000	-0.817410000	-1.441304000
B	1.234744000	-0.000000000	-0.654157000
B	0.803444000	-1.638074000	-0.126382000
Li	-0.000000000	-1.539232000	1.861469000
B	1.985142000	-0.773633000	0.615672000
B	-0.803444000	-1.638074000	-0.126382000

14

F-Li

B	1.266036000	0.398199000	-0.000000000
Li	0.684254000	2.605688000	-0.000000000
B	0.582602000	0.966754000	1.440013000
B	-0.948677000	1.285703000	0.824257000
B	-0.948677000	1.285703000	-0.824257000
B	0.582602000	0.966754000	-1.440013000
B	-0.753070000	-0.169530000	-1.535393000
B	0.913760000	-0.622595000	-1.390279000
B	-0.488249000	-1.595859000	-0.784667000
B	1.073889000	-1.427953000	0.000000000
B	-0.488249000	-1.595859000	0.784667000
B	0.913760000	-0.622595000	1.390279000
B	-0.753070000	-0.169530000	1.535393000
Li	-2.272015000	-0.437675000	0.000000000

14

A-Na

B	0.620589000	0.397745000	0.828535000
Na	0.912349000	2.879410000	0.000000000
B	0.620589000	0.397745000	-0.828535000
B	0.947792000	-1.046742000	-0.000000000
B	0.613132000	-1.215937000	1.720671000
B	-0.102233000	0.087819000	2.317025000
B	-0.904484000	1.141231000	1.496927000
B	0.907596000	-2.506125000	-0.774005000
B	0.907596000	-2.506125000	0.774005000
Na	-1.813962000	-1.165041000	-0.000000000
B	-1.233446000	1.465666000	0.000000000
B	-0.904484000	1.141231000	-1.496927000
B	-0.102233000	0.087819000	-2.317025000
B	0.613132000	-1.215937000	-1.720671000

14

D-Na

B	0.690848000	0.121075000	0.724982000
Na	3.031996000	-0.585268000	-0.108933000
B	1.162447000	1.653138000	0.168258000
B	1.061404000	0.674230000	-1.080654000
B	0.539496000	-0.881957000	-1.131049000
B	0.526493000	-1.564439000	0.360985000
B	-0.916777000	0.419512000	1.744888000
B	-0.067776000	1.691672000	1.167212000
B	-1.749738000	0.997081000	0.419696000
B	-1.921778000	0.958103000	-1.143303000

B	-0.424937000	1.515334000	-0.623227000
B	-0.711133000	0.084450000	-1.642604000
B	-0.222594000	-1.039996000	1.626779000
Na	-2.107430000	-1.518460000	-0.160141000

14

E-Na

B	0.804792000	1.635278000	-0.573365000
B	1.239854000	-0.000000000	-1.113562000
B	-0.000000000	-0.819484000	-1.889097000
B	-0.804792000	-1.635278000	-0.573365000
B	-2.030575000	-0.776068000	0.120343000
B	-2.030575000	0.776068000	0.120343000
B	-0.804792000	1.635278000	-0.573365000
Na	0.000000000	-1.889294000	1.776683000
B	-1.239854000	0.000000000	-1.113562000
B	2.030575000	0.776068000	0.120343000
B	2.030575000	-0.776068000	0.120343000
Na	0.000000000	1.889294000	1.776683000
B	0.000000000	0.819484000	-1.889097000
B	0.804792000	-1.635278000	-0.573365000

14

C-Na

B	0.000000000	1.606478000	0.772158000
Na	0.000000000	0.000000000	2.860783000
B	0.803239000	1.391251000	-0.772158000
B	1.606478000	-0.000000000	-0.772158000
B	1.391251000	-0.803239000	0.772158000
B	1.391251000	0.803239000	0.772158000
B	-1.391251000	0.803239000	0.772158000
B	-1.606478000	0.000000000	-0.772158000
B	-0.803239000	1.391251000	-0.772158000
Na	0.000000000	0.000000000	-2.860783000
B	0.803239000	-1.391251000	-0.772158000
B	-0.000000000	-1.606478000	0.772158000
B	-1.391251000	-0.803239000	0.772158000
B	-0.803239000	-1.391251000	-0.772158000

14

F-Na

B	0.911605000	1.194372000	0.000003000
Na	2.938308000	-0.672862000	-0.000009000
B	1.024643000	0.275794000	-1.419235000
B	0.450511000	-1.189605000	-0.826047000
B	0.450514000	-1.189611000	0.826034000
B	1.024649000	0.275782000	1.419234000

B	-0.672216000	-0.230912000	1.528392000
B	-0.128899000	1.418332000	1.392288000
B	-1.719010000	0.787669000	0.786047000
B	-0.715573000	1.993737000	0.000010000
B	-1.719012000	0.787673000	-0.786031000
B	-0.128905000	1.418345000	-1.392276000
B	-0.672222000	-0.230899000	-1.528393000
Na	-2.077438000	-1.741082000	-0.000003000

14

A-K -15.3

B	1.353664000	-0.780087000	0.000000000
B	1.900279000	-2.129839000	0.773384000
B	0.529510000	0.441462000	-0.827820000
B	1.900279000	-2.129839000	-0.773384000
B	-1.131099000	0.668252000	-1.500135000
B	1.111778000	-1.051988000	-1.714863000
K	-1.393285000	-2.187561000	0.000000000
B	-0.035653000	-0.096102000	-2.308538000
B	0.529510000	0.441462000	0.827820000
B	1.111778000	-1.051988000	1.714863000
K	0.184605000	3.295831000	0.000000000
B	-1.131099000	0.668252000	1.500135000
B	-0.035653000	-0.096102000	2.308538000
B	-1.510307000	0.905094000	0.000000000

14

D-K

B	0.664814000	0.277862000	0.685722000
K	3.282367000	-0.758000000	-0.063143000
B	1.297883000	1.743305000	0.093283000
B	1.057546000	0.737759000	-1.112693000
B	0.347509000	-0.741470000	-1.103518000
B	0.273324000	-1.378697000	0.402543000
B	-0.884762000	0.819182000	1.747234000
B	0.114652000	1.948760000	1.122902000
B	-1.678799000	1.431972000	0.416077000
B	-1.870379000	1.414239000	-1.145688000
B	-0.311365000	1.778184000	-0.658747000
B	-0.804507000	0.345510000	-1.600687000
B	-0.357600000	-0.714350000	1.664462000
K	-2.716135000	-1.258383000	-0.071302000

14

E-K

B	-0.803703000	1.627665000	-0.969801000
B	-0.000000000	0.820517000	-2.298681000

B	1.246931000	-0.000000000	-1.532843000
B	0.803703000	-1.627665000	-0.969801000
B	-0.803703000	-1.627665000	-0.969801000
B	-2.055255000	-0.776768000	-0.313727000
B	-2.055255000	0.776768000	-0.313727000
B	2.055255000	0.776768000	-0.313727000
B	-1.246931000	0.000000000	-1.532843000
K	-0.000000000	2.251973000	1.683836000
B	-0.000000000	-0.820517000	-2.298681000
B	0.803703000	1.627665000	-0.969801000
K	-0.000000000	-2.251973000	1.683836000
B	2.055255000	-0.776768000	-0.313727000

14

C-K

B	-1.604906000	0.000000000	0.775017000
K	0.000000000	0.000000000	3.289526000
B	-1.390005000	0.802395000	-0.774682000
B	0.000000000	1.604906000	-0.775017000
B	0.802395000	1.390005000	0.774682000
B	-0.802395000	1.390005000	0.774682000
B	-0.802395000	-1.390005000	0.774682000
B	-0.000000000	-1.604906000	-0.775017000
B	-1.390005000	-0.802395000	-0.774682000
K	0.000000000	0.000000000	-3.289526000
B	1.390005000	0.802395000	-0.774682000
B	1.604906000	0.000000000	0.775017000
B	0.802395000	-1.390005000	0.774682000
B	1.390005000	-0.802395000	-0.774682000

14

F-K

B	0.995833000	1.334854000	0.000004000
K	3.187416000	-0.878038000	-0.000009000
B	0.994034000	0.425794000	-1.428467000
B	0.261504000	-0.959038000	-0.826610000
B	0.261506000	-0.959046000	0.826601000
B	0.994038000	0.425781000	1.428468000
B	-0.759861000	0.123154000	1.504417000
B	-0.010309000	1.700670000	1.395637000
B	-1.676142000	1.272387000	0.784993000
B	-0.521863000	2.338037000	0.000011000
B	-1.676146000	1.272397000	-0.784980000
B	-0.010312000	1.700682000	-1.395621000
B	-0.759866000	0.123168000	-1.504411000
K	-2.685420000	-1.437446000	-0.000003000

14

A-Rb

B	0.641381000	0.401233000	0.827863000
B	0.182533000	-0.219312000	2.309841000
B	-1.432816000	0.522861000	0.000000000
B	1.479186000	-0.961377000	1.714316000
Rb	-0.147627000	3.349058000	0.000000000
B	-1.029022000	0.349152000	1.502931000
B	2.454678000	-1.878383000	0.773614000
Rb	-0.891188000	-2.706853000	0.000000000
B	1.662533000	-0.657802000	0.000000000
B	1.479186000	-0.961377000	-1.714316000
B	2.454678000	-1.878383000	-0.773614000
B	0.182533000	-0.219312000	-2.309841000
B	0.641381000	0.401233000	-0.827863000
B	-1.029022000	0.349152000	-1.502931000

14

D-Rb

B	0.621457000	0.572598000	0.675904000
Rb	3.359115000	-0.644279000	-0.031326000
B	1.310351000	2.007021000	0.065333000
B	1.023583000	0.993834000	-1.121689000
B	0.244208000	-0.448946000	-1.095952000
B	0.146594000	-1.066437000	0.417195000
B	-0.898989000	1.198946000	1.747833000
B	0.147713000	2.271895000	1.102984000
B	-1.678312000	1.821960000	0.413488000
B	-1.874913000	1.811283000	-1.148968000
B	-0.300342000	2.103920000	-0.674209000
B	-0.871010000	0.677260000	-1.588968000
B	-0.435861000	-0.357144000	1.678103000
Rb	-3.012423000	-0.921422000	-0.032330000

14

E-Rb

B	-0.803975000	1.625112000	1.492128000
B	1.250054000	-0.000000000	2.064114000
B	-2.066943000	0.777041000	0.852169000
B	2.066943000	0.777041000	0.852169000
Rb	-0.000000000	2.411939000	-1.294136000
B	0.803975000	1.625112000	1.492128000
B	-0.000000000	0.821346000	2.823900000
B	2.066943000	-0.777041000	0.852169000
B	-0.000000000	-0.821346000	2.823900000
B	-1.250054000	0.000000000	2.064114000

B	-0.803975000	-1.625112000	1.492128000
Rb	-0.000000000	-2.411939000	-1.294136000
B	-2.066943000	-0.777041000	0.852169000
B	0.803975000	-1.625112000	1.492128000

14

C-Rb

B	0.000000000	1.604812000	0.775600000
Rb	0.000000000	0.000000000	3.489954000
B	0.802406000	1.389808000	-0.775600000
B	1.604812000	-0.000000000	-0.775600000
B	1.389808000	-0.802406000	0.775600000
B	1.389808000	0.802406000	0.775600000
B	-1.389808000	0.802406000	0.775600000
B	-1.604812000	0.000000000	-0.775600000
B	-0.802406000	1.389808000	-0.775600000
Rb	0.000000000	0.000000000	-3.489954000
B	0.802406000	-1.389808000	-0.775600000
B	-0.000000000	-1.604812000	0.775600000
B	-1.389808000	-0.802406000	0.775600000
B	-0.802406000	-1.389808000	-0.775600000

14

F-Rb

B	1.008020000	1.650982000	0.000012000
Rb	3.265504000	-0.748151000	-0.000007000
B	0.959579000	0.735207000	-1.424130000
B	0.157120000	-0.611405000	-0.826632000
B	0.157121000	-0.611417000	0.826622000
B	0.959580000	0.735185000	1.424141000
B	-0.810481000	0.522749000	1.500834000
B	0.022630000	2.060312000	1.396307000
B	-1.665432000	1.722038000	0.785384000
B	-0.454959000	2.722921000	0.000020000
B	-1.665431000	1.722047000	-0.785355000
B	0.022629000	2.060333000	-1.396277000
B	-0.810481000	0.522771000	-1.500828000
Rb	-2.979003000	-1.039920000	-0.000006000

14

A-Cs

B	0.699046000	0.367611000	0.829121000
B	0.287269000	-0.288138000	2.304871000
B	-1.363858000	0.400907000	0.000000000
B	1.646798000	-0.916224000	1.712230000
Cs	-0.187724000	3.396127000	0.000000000
B	-0.955727000	0.218383000	1.500939000

B	2.713169000	-1.733053000	0.773172000
Cs	-0.650918000	-2.950841000	0.000000000
B	1.807809000	-0.596211000	0.000000000
B	1.646798000	-0.916224000	-1.712230000
B	2.713169000	-1.733053000	-0.773172000
B	0.287269000	-0.288138000	-2.304871000
B	0.699046000	0.367611000	-0.829121000
B	-0.955727000	0.218383000	-1.500939000

14

D-Cs

B	0.600899000	0.754405000	0.665630000
Cs	3.437240000	-0.538979000	-0.020862000
B	1.312216000	2.177461000	0.052845000
B	0.999743000	1.162356000	-1.127114000
B	0.192432000	-0.264984000	-1.091087000
B	0.089051000	-0.873519000	0.423138000
B	-0.907396000	1.419464000	1.747649000
B	0.163574000	2.464809000	1.098765000
B	-1.680901000	2.049719000	0.412244000
B	-1.879914000	2.044916000	-1.149650000
B	-0.298362000	2.302248000	-0.677856000
B	-0.901647000	0.883433000	-1.579999000
B	-0.471783000	-0.144477000	1.681975000
Cs	-3.184323000	-0.731552000	-0.020642000

14

E-Cs

B	-0.804365000	1.623783000	1.838748000
B	1.249855000	-0.000000000	2.415714000
B	-2.066612000	0.776813000	1.202684000
B	2.066612000	0.776813000	1.202684000
Cs	0.000000000	2.434945000	-1.061068000
B	0.804365000	1.623783000	1.838748000
B	0.000000000	0.821762000	3.173165000
B	2.066612000	-0.776813000	1.202684000
B	-0.000000000	-0.821762000	3.173165000
B	-1.249855000	0.000000000	2.415714000
B	-0.804365000	-1.623783000	1.838748000
Cs	-0.000000000	-2.434945000	-1.061068000
B	-2.066612000	-0.776813000	1.202684000
B	0.804365000	-1.623783000	1.838748000

14

C-Cs

B	1.605000000	-0.000000000	0.775482000
Cs	0.000000000	0.000000000	3.619639000

B	1.389975000	-0.802405000	-0.775305000
B	-0.000000000	-1.605000000	-0.775482000
B	-0.802405000	-1.389975000	0.775305000
B	0.802405000	-1.389975000	0.775305000
B	0.802405000	1.389975000	0.775305000
B	0.000000000	1.605000000	-0.775482000
B	1.389975000	0.802405000	-0.775305000
Cs	-0.000000000	-0.000000000	-3.619639000
B	-1.389975000	-0.802405000	-0.775305000
B	-1.605000000	-0.000000000	0.775482000
B	-0.802405000	1.389975000	0.775305000
B	-1.389975000	0.802405000	-0.775305000

14

F-Cs

B	1.000611000	1.800642000	0.000013000
Cs	3.350794000	-0.622159000	-0.000005000
B	0.937160000	0.937011000	-1.451949000
B	0.123974000	-0.388589000	-0.826883000
B	0.123975000	-0.388601000	0.826877000
B	0.937161000	0.936989000	1.451962000
B	-0.838815000	0.759207000	1.484453000
B	0.034200000	2.283593000	1.398307000
B	-1.669862000	1.980103000	0.783881000
B	-0.430857000	2.952004000	0.000022000
B	-1.669862000	1.980114000	-0.783850000
B	0.034200000	2.283615000	-1.398274000
B	-0.838816000	0.759229000	-1.484442000
Cs	-3.145618000	-0.822870000	-0.000005000